UNIVERSITÀ DEGLI STUDI DI PADOVA

DIPARTIMENTO DI MATEMATICA

SCUOLA DI DOTTORATO DI RICERCA IN : SCIENZE MATEMATICHE
INDIRIZZO : MATEMATICA
CICLO XXIX

FRACTIONAL CALCULUS:
NUMERICAL METHODS AND SIR MODELS

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January 2017

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Abstract

Fractional calculus is [168] "the theory of integrals and derivatives of arbitrary order, which unify and generalize the notions of integer-order differentiation and n-fold integration". The idea of generalizing differential operators to a non-integer order, in particular to the order $1/2$, first appears in the correspondence of Leibniz with L'Hopital (1695), Johann Bernoulli (1695), and John Wallis (1697) as a mere question or maybe even play of thoughts. In the following three hundred years a lot of mathematicians contributed to the fractional calculus: Laplace (1812), Lacroix (1812), Fourier (1822), Abel (1823-1826), Liouville (1832-1837), Riemann (1847), Grünwald (1867-1872), Letnikov (1868-1872), Sonin (1869), Laurent (1884), Heaviside (1892-1912), Weyl (1917), Davis (1936), Erdèlyi (1939-1965), Gelfand and Shilov (1959-1964), Dzherbashian (1966), Caputo (1969), and many others. Yet, it is only after the First Conference on Fractional Calculus and its applications that the fractional calculus becomes one of the most intensively developing areas of mathematical analysis. Recently, many mathematicians and applied researchers have tried to model real processes using the fractional calculus. This is because of the fact that the realistic modeling of a physical phenomenon does not depend only on the instant time, but also on the history of the previous time which can be successfully achieved by using fractional calculus. In other words, the nature of the definition of the fractional derivatives have provided an excellent instrument for the modeling of memory and hereditary properties of various materials and processes.

Outline of the thesis

In this thesis several aspects of fractional calculus will be presented ranging from its history over analytical and numerical results to SIR models. Such models have become very important for decision-making about infectious disease intervention programs. Main claim is that a fractional model can give a more realistic interpretation of natural phenomena. Generalized SIR models are presented in this thesis by using ordinary differential equations of fractional order. This thesis is structured as follows:

The thesis begins in Chapter 1 with some well known analytical and numerical results on classical calculus are stated. One reason behind this is due to the fact that those results are needed for several proofs of theorems in later chapters and thus they are stated here for completeness. Moreover, classical calculus can be regarded as a special case of fractional calculus, since results in fractional calculus should contain the classical case in a certain way. Also in

Chapter 1 some well known results on integral transforms and special functions are stated. In general, the results of that chapter will be used frequently in the succeeding chapters dealing with the analytical and numerical theory of fractional calculus.

Chapter 2 begins with a brief historical review of the theory of fractional calculus. The basic definitions and properties of fractional integrals and derivatives are introduced, including the most frequently used Riemann-Liouville integral, the Riemann-Liouville derivative, the Caputo derivative, and Grünwald-Letnikov derivative. Also, all the important results for the properties of Riemann-Liouville and Caputo fractional derivatives are summarized in a special chart. Analytical results of differential equations of fractional order are presented in this chapter. Most of the stated results can be found in similar form in textbooks on fractional calculus, but some of the presented results give additional properties. Finally, a brief introduction of mathematical modeling of infectious diseases are presented including those of fractional order.

In Chapter 3, numerical methods for fractional integrals and fractional derivatives are displayed in detail. We first derive the numerical schemes based on linear multistep methods for the fractional integrals (i.e. Riemann-Liouville integrals). Then we investigate the Grünwald-Letnikov approximation for the fractional order differential equation of Caputo type. Also, The natural generalization of the above methods are introduced.

In the next chapter, we derive another numerical method, which is also based on fractional linear multistep methods, more precisely we formulate the well known classical Adams-Moulton-Bashforth method in the fractional setting. For the error analysis of this algorithm and some important examples are also presented within this chapter.

In Chapter 5 the presented numerical methods are employed for two fractional-order SIR models and the theoretical results of Chapter 4 are verified. In addition some of the theoretical analysis are shown to confirm the numerical results.

Remarks

Some new results in this thesis are included in new papers as follows:

Article title	Journal title	Received	Current status
The solution of fractional order epidemic model by implicit Adams methods	Appl Math Model	30 Apr 2015	Published (24 Dec 2016)
The effect of vaccination and treatment of measles disease described by a fractional order model	Journal of Math & Computational Sci (JMCS)	19 Aug 2016	In Editing (10 Oct 2016)

Sommario

Il calcolo frazionario è [168] "the theory of integrals and derivatives of arbitrary order, which unify and generalize the notions of integer-order differentiation and n-fold integration". L' idea di generalizzare operatori differenziali ad un ordine non intero, in particolare di ordine $1/2$, compare per la prima volta in una corrispondenza di Leibniz con L'Hopital (1695), Johann Bernoulli (1695), e John Wallis (1697), come una semplice domanda o forse un gioco di pensieri. Nei successivi trecento anni molti matematici hanno contribuito al calcolo frazionario: Laplace (1812), Lacroix (1812), di Fourier (1822), Abel (1823-1826), Liouville (1832-1837), Riemann (1847), Grünwald (1867-1872), Letnikov (1868-1872), Sonin (1869), Laurent (1884), Heaviside (1892-1912), Weyl (1917), Davis (1936), Erdèlyi (1939-1965), Gelfand e Shilov (1959-1964), Dzherbashian (1966), Caputo (1969), e molti altri. Eppure, è solo dopo la prima conferenza sul calcolo frazionario e le sue applicazioni che questo tema diventa una delle le aree più intensamente studiate dell'analisi matematica. Recentemente, molti matematici e ingegneri hanno cercato di modellare i processi reali utilizzando il calcolo frazionario. Questo a causa del fatto che spesso, la modellazione realistica di un fenomeno fisico non è locale nel tempo, ma dipende anche dalla storia, e questo comportamento può essere ben rappresentato attraverso modelli basati sul calcolo frazionario. In altre parole, la defnizione dei derivata frazionaria fornisce un eccellente strumento per la modellazione della memoria e delle proprietà ereditarie di vari materiali e processi.

In questa tesi diversi aspetti del calcolo frazionario saranno presentati, partendo dalla storia, fino ai risultati analitici e numerici e ai modelli SIR. Tali modelli sono diventati molto importanti per il processo decisionale sui programmi di intervento sulle malattie infettive. Il punto chiave è che un modello frazionario può dare un'interpretazione più realistica dei fenomeni naturali. Il modello SIR generalizzato viene presentato in questa tesi utilizzando equazioni differenziali di tipo frazionario. Questa tesi è strutturato come segue:

La tesi inizia nel Capitolo 1 con alcuni risultati analitici e numerici ben noti del calcolo. La ragione è dovuta al fatto che tali risultati sono necessari per atri risultati nei capitoli successivi e quindi, per completezza, sono stati riportati. Inoltre, il calcolo classico può essere considerato come un caso particolare di calcolo frazionario, dal momento che i risultati nel calcolo frazionario devono contenere il caso classico in un certo modo. Nel Capitolo 1 alcuni risultati ben noti sulla trasformate integrali e funzioni speciali sono riportati. In generale, i risultati di questo capitolo saranno utilizzati frequentemente nei capitoli successivi.

Il Capitolo 2 inizia con una breve rivisitazione storica della teoria del calcolo frazionario.

Le principali definizioni e le proprietà degli integrali e delle derivate frazionarie vengono qui introdotte, comprese le definizioni di integrale di Riemann-Liouville, derivata di Riemann-Liouville, derivata di Caputo e di Grünwald-Letnikov. Inoltre, tutti i risultati importanti riguardo le proprietà delle derivate di Riemann-Liouville e Caputo sono riassunti in una tabella. Alcuni risultati analitici sulle equazioni dufferenziali di ordine frazionario sono presentati in questo capitolo. La maggior parte dei risultati riportati si possono trovare in forma simile nei libri di testo sul calcolo frazionario, ma alcuni dei risultati presentati forniscono proprietà aggiuntive. Infine, viene presentata una breve introduzione sulla modellazione dello sviluppo delle malattie infettive attraverso il calcolo frazionario.

Nel Capitolo 3, vengono presentati alcuni metodi numerici per integrali e derivate frazionarie. Per prima cosa vengono introdotti gli schemi numerici basati sui metodi multistep lineari per gli integrali frazionari (cioè integrali di Riemann-Liouville). Poi viene studiata l'approssimazione di Grünwald-Letnikov della derivata frazionaria per la risoluzione numerica di equazioni differenziali di tipo Caputo.

Nel capitolo successivo, viene introdotto un altro metodo numerico, sempre basato sui metodi multistep per equazioni frazionarie. In particolare viene presentato il noto Adams-Moulton-Bashforth nell'impostazione frazionaria. L'analisi di errore di questo schema insieme ad alcuni importanti esempi vengono riportati in questo capitolo.

Nel Capitolo 5 i metodi numerici presentati sono impiegati per la risoluzione numerica di due modelli SIR frazionari. Inoltre vengono numericamente verificati i risultati teorici del Capitolo 4. I risultati numerici vengono anche confrontati con quelli attesi dalla teoria.

To My Sons

Acknowledgements

Ismail Gad Ameen Abdelsheed
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Chapter 1

Preliminaries

1.1 Integer calculus

Integer calculus is used in various mathematical fields and results can be found in numerous books on analysis, differentiation and integration, differential equations, integral equations etc. Often, these results can be carried over to the fractional case. So, the important results of integer calculus are outlined in this section. Also, we consider results on ordinary differential equations (ODEs) and explain a class of numerical methods frequently used to solve them.

1.1.1 Integration and differentiation

The fundamental theorem of classical calculus ([154], Theorem 6.18) given a relation between integer order integration and differentiation.

Theorem 1.1.1. *(Fundamental Theorem of Classical Calculus) Let $f : [a,b] \to \mathbb{R}$ be a continuous function and let $F : [a,b] \to \mathbb{R}$ be defined by*

$$F(t) = \int_a^t f(s)ds.$$

Then, F is differentiable and

$$F' = f.$$

It is one of the goals of fractional calculus to retain this relation in a generalized sense. Throughout this thesis, It is convenient to use the following notations from now on.

Definition 1.1.2. 1. By D, we denote the operator that maps a differentiable function onto its derivative, i.e.

$$Df(t) := f'(t) = \frac{d}{dt}f(t).$$

2. By I_a, we denote the operator that maps a function f, assumed to be (Riemann) integrable on the compact interval $[a, b]$, onto its primitive centered at a, i.e.

$$I_a f(t) := \int_a^t f(s)ds, \qquad (1.1)$$

for $a \leq t \leq b$. If $a = 0$ we will simply write I instead of I_0.

3. For $n \in \mathbb{N}$ we use the symbols D^n and I_a^n to denote the $n-$fold iterates of D and I_a, respectively, i.e. we set $D^1 := D$, $I_a^1 := I_a$, and $D^n := DD^{n-1}$ and $I_a^n := I_a I_a^{n-1}$ for $n \geq 2$.

A first result, which will be most important for the later generalization to non-integer integrals (i.e. fractional integrals), can be obtained from this definition. We now begin with the integral operator I_a^n. In the case $n \in \mathbb{N}$, it is well known (and easily proved by induction) (see e.g. [155]) that we can replace the recursive definition of Definition 1.1.2 3. by the following explicit formula.

Lemma 1.1.3. *Let f be Riemann integrable on $[a, b]$. Then, for $a \leq t \leq b$ and $n \in \mathbb{N}$, we have*

$$I_a^n f(t) = \frac{1}{(n-1)!} \int_a^t (t-s)^{n-1} f(s)ds.$$

From this Lemma another consequence can be drawn. In terms of Definition 1.1.2 the fundamental theorem of classical calculus reads $DI_a f = f$, which implies by Definition 1.1.2 3. that $D^n I_a^n f = f$. This leads to the following Lemma:

Lemma 1.1.4. *Let $m, n \in \mathbb{N}$ such that $m > n$, and let $f(t)$ be a function having a continuous nth derivative on the interval $[a, b]$. Then,*

$$D_a^n f(t) = D^m I_a^{m-n} f(t). \qquad (1.2)$$

Before stating additional properties of integral and differential operators it is necessary to introduce some classical function spaces as follow:

Definition 1.1.5. Let $k \in \mathbb{N}$ and $1 \leq p$. We define:

$$
\begin{aligned}
L_p[a, b] &:= \left\{ f : [a, b] \rightarrow \mathbb{R}; f \text{ is measurable on } [a, b] \text{ and } \int_a^b |f(t)|^p dt < \infty \right\}, \\
C^k[a, b] &:= \{ f : [a, b] \rightarrow \mathbb{R}; f \text{ has a continuous } k\text{th derivative} \}, \\
C[a, b] &:= C^0[a, b],
\end{aligned}
$$

For $1 \leq p \leq \infty$ the function space $L_p[a, b]$ is the usual Lebesgue space and the Fundamental Theorem 1.1.1 in the Lebesgue space as follows:

Theorem 1.1.6. (Fundamental Theorem in Lebesgue Space) *Let $f \in L_1[a, b]$. Then, $I_a f$ is differentiable almost everywhere in $[a, b]$, and $DI_a f = f$ also holds almost everywhere on $[a, b]$.*

Another important basic result in classical analysis is Taylor's theorem. Instead of using the classical formulation we give a more instructive definition. To do this, we shall also introduce another function space :

Definition 1.1.7. By A^n or $A^n[a,b]$ we denote the set of functions with an absolutely continuous $(n-1)$st derivative, i.e. the functions f for which there exists (almost everywhere) a function $g \in L_1[a,b]$ such that

$$f^{(n-1)}(t) = f^{(n-1)}(a) + \int_a^t g(s)ds.$$

In this case we call g the (generalized) nth derivative of f, and we simply write $g = f^{(n)}$.

Theorem 1.1.8. (*Taylor expansion*) *For* $m \in \mathbb{N}$ *the following statements are equivalent:*

1. $f \in A^m[a,b]$.

2. *For every* $t, s \in [a,b]$,

$$f(t) = \sum_{k=0}^{m-1} \frac{(t-s)^k}{k!} D^k f(s) + I_s^m D^m f(t).$$

An important part of the Taylor expansion is its polynomial:

Definition 1.1.9. Let $f(t) \in C^n[a,b]$ and $t_0 \in [a,b]$. The polynomial

$$T_n[f, t_0](t) = \sum_{k=0}^{n} \frac{(t-t_0)^k}{k!} D^k f(t_0),$$

is called *the Taylor polynomial of order* n, centered at t_0.

For some proofs in later chapters we will need the following important theorems:

Theorem 1.1.10. (*Fubini's Theorem*) *Let* $[a,b]$ *and* $[c,d]$ *be two compact intervals,* f *be a Riemann-integrable function and assume that*

$$g(s) = \int_a^b f(t,s)ds \quad \text{exists for every fixed} \quad s \in [c,d].$$

Then, g *is Riemann-integrable on* $[c,d]$ *and*

$$\int_{[a,b]\times[c,d]} f(t,s)d(t,s) = \int_c^d \left(\int_a^b f(t,s)dt \right) ds.$$

If furthermore

$$h(y) = \int_c^d f(t,s)ds \quad \text{exists for every fixed} \quad t \in [a,b]$$

then

$$\int_a^b \left(\int_c^d f(t,s)ds \right)dt = \int_c^d \left(\int_a^b f(t,s)dt \right)ds = \int_{[a,b]\times[c,d]} f(t,s)d(t,s).$$

We now state some important fixed point theorems which we are need it in the upcoming Subsection 2.2.2. We start with the generalization of Banach's fixed point theorem that we take from [174]:

Theorem 1.1.11. (Weissinger's Fixed Point Theorem) *Assume (U,d) to be a nonempty complete metric space, and let $\epsilon_j \geq 0$ for every $j \in \mathbb{N}_0$ and such that $\sum_{j=0}^{\infty} \epsilon_j$ converges. Moreover, let the mapping $A : U \to U$ satisfy the inequality*

$$d(A^j u, A^j v) \leq \epsilon_j d(u,v),$$

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

An immediate consequence is the following theorem:

Theorem 1.1.12. (Banach's Fixed Point Theorem) *Assume (U,d) to be a nonempty complete metric space, let $0 \leq \epsilon < 1$, and let the mapping $A : U \to U$ satisfy the inequality*

$$d(Au, Av) \leq \epsilon d(u,v),$$

for every $u,v \in U$. Then, A has a uniquely determined fixed point u^*. Furthermore, for any $u_0 \in U$, the sequence $(A^j u_0)_{j=1}^{\infty}$ converges to this fixed point u^*.

For the uniqueness of a fixed point we have Schauder's theorem (see e.g. [28]).

Theorem 1.1.13. (Schauder's Fixed Point Theorem) *Let (E,d) be a complete metric space, let U be a closed convex subset of E, and let $A : U \to U$ be a mapping such that the set $\{Au : u \in U\}$ is relatively compact in E. Then A has got at least one fixed point.*

In this context we recall a definition:

Definition 1.1.14. Let (E,d) be a metric space and $F \subseteq E$. The set F is called relatively compact in E if the closure of F is a compact subset of E.

A helpful classical result from Analysis in connection with such sets is as follows. The proof can be found in many standard textbooks, e.g. in ([29], p.30].

Theorem 1.1.15. (Arzelà-Ascoli) *Let $F \subseteq C[a,b]$ for some $a < b$, and assume the sets to be equipped with the Chebyshev norm. Then, F is relatively compact in $C[a,b]$ if F is equicontinuous (i.e. for every $\varepsilon > 0$ there exists some $\delta > 0$ such that for all $f \in F$ and all $t, t^* \in [a,b]$ with $|t - t^*| < \delta$ we have $|f(t) - f(t^*)| < \varepsilon$) and uniformly bounded (i.e. there exists a constant $C > 0$ such that $\|f\|_{\infty} \leq C$ for every $f \in F$).*

We now consider results on ODEs in the next subsection and explain a class of numerical methods frequently used to solve them.

1.1.2 Linear multistep methods for an ODE of first order

Here, we give some important results for the theory of ordinary differential equations and in addition explain the idea of multistep methods. These results will formulate in later chapters for the fractional case. We begin with a formal definition of an ODE

Definition 1.1.16. Let $n \in \mathbb{N}$ and $f : A \subseteq \mathbb{R}^2 \to \mathbb{R}$. Then

$$D^n y(t) = f(t, y(t)), \tag{1.3}$$

is called ordinary differential equation of order n. If additionally initial conditions of the form

$$D^k y(0) = y_0^{(k)} = b_k, \quad (k = 0, 1, 2, ..., n - 1) \tag{1.4}$$

are defined we understand the differential equation (1.3), equipped with initial conditions (1.4) as initial value problem (IVP).

A first result, which will become fundamental for the fractional case is the equivalence of an ODE to an integral equation, given in the following lemma:

Lemma 1.1.17. *The function $y(t)$ is a solution to the differential equation (1.3) equipped with initial condition (1.4) if and only if $y(t)$ is a solution of the integral equation*

$$y(t) = \sum_{k=0}^{n-1} \frac{x^k}{k!} D^k y(0) + \frac{1}{(n-1)!} \int_0^t (t-s)^{n-1} f(s, y(s)) dt. \tag{1.5}$$

The question of existence and uniqueness of a solution of an ODE (1.3) equipped with initial conditions (1.4) is answered by the classical theorems of Peano and Picard-Lindelöf.

Before we state the main property of the solution of IVP (1.3)-(1.4), we want the following definition:

Definition 1.1.18. Let $n \in \mathbb{N}$, $G \subseteq \mathbb{R}^n$ and $f \in C(G)$. Then the function f is called analytic in G, if for any point $(\nu_1, \nu_2, ..., \nu_n) \in G$ there exists a power series satisfying

$$f(t_1, t_2, ..., t_n) = \sum_{\mu_1, ..., \mu_n = 0}^{\infty} c_{\mu_1, ..., \mu_n} (t - \nu_1)^{\mu_1} (t - \nu_2)^{\mu_2} ... (t - \nu_n)^{\mu_n},$$

which is absolutely convergent in a neighbourhood of $(\nu_1, \nu_2, ..., \nu_n)$.

Thus, we can state the following theorem:

Theorem 1.1.19. *If the function f of the differential equation (1.3) equipped with initial conditions (1.4) is analytic in a neighbourhood of $(0, Dy(0), ..., D^n y(0))$, the solution of (1.3) is analytic in a neighbourhood of 0.*

The question of differentiability of the solution can also be assured for ODEs:

Theorem 1.1.20. *Let $k \in \mathbb{N}$, $b > 0$ and $f \in C^k([0, b] \times \mathbb{R})$. Then the solution of the initial value problem*

$$Dy(t) = f(t, y(t)), \quad y(0) = y_0 = b_0 \tag{1.6}$$

is $(k + 1)$-times differentiable.

In the next part, we are interested in a numerical method for solving a first order differential equation with a given initial condition. This means we are interested in a solution y on a closed interval $[0, T]$ for some $T > 0$. In general numerical methods do not produce a solution on the whole interval in question, but rather give the solution on a prescribed set of nodes in the interval. Therefore we assume from now on that the nodes are arranged equispaced inside the interval $[0, T]$ and on its border with a given step-size h. Additionally the nodes are assumed to be numbered increasingly $t_0, t_1, ..., t_N$, where $N = T/h$, $t_0 = 0$ and $t_N = T$. Furthermore, we denote by y_m the approximation of $y(t_m)$ and equally $f_m = f(t_m, y_m)$ as discretized right hand side of the differential equation in question. In this setting we can formulate a definition of a linear multistep method (LMM):

Definition 1.1.21. We define a linear multistep method for an ODE of first order (i.e. $n = 1$ in (1.3)) by

$$\sum_{k=-1}^{p} \beta_k y_{m-k} = h \sum_{k=-1}^{p} \gamma_k f(t_{m-k}, y_{m-k}), \tag{1.7}$$

where β_k, γ_k for $k = -1, 0, 1, ..., p$ denote real constants.

Definition 1.1.22. Given a LMM (1.7), the polynomial

$$\rho(\zeta) = \sum_{k=-1}^{p} \beta_k \zeta^{p-k}, \quad \sigma(\zeta) = \sum_{k=-1}^{p} \gamma_k \zeta^{p-k},$$

are called the first and second characteristic polynomial, respectively.

From now on we will say linear multistep method of type (ρ, σ) to denote the structure of the method. By Lemma 1.1.17 we have the equivalence between ODE (1.3) and Volterra integral equation (1.5). Thus we applied a LMM (ρ, σ) to an integral equation as follow:

Lemma 1.1.23. *A linear multistep method (ρ, σ) applied to the integral equation*

$$y(t) = \int_0^t f(s)ds,$$

can be described as convolution quadrature:

$$({}_h I f)(t) = h \sum_{j=0}^{m} \omega_{m-j} f(jh), \quad t = mh.$$

Here $_hI$ denotes the discretization of step length h for the integral operator I. The convolution weights ω_m are given by the power series of the generating function ω defined by

$$\omega(\zeta) = \frac{\sigma(1/\zeta)}{\rho(1/\zeta)}. \tag{1.8}$$

Proof. This lemma is a specific case of Lemma 2.1 in [112]. $\qquad\qquad\square$

In ([83], Ch. 5.2-3) the following definition can be found for the convergence of a LMM (ρ, σ).

Definition 1.1.24. Let $f(t, y)$ defined for all $t \in [0, T]$ so that the initial value problem (1.6) is uniquely solvable for all b_0. A linear multistep method (ρ, σ) is then called convergent if

$$\lim_{\substack{h \to 0 \\ t_m = t}} y_m = y(t)$$

holds for all $t \in [0, T]$ and all solutions $\{y_m\}$ of the difference equation (1.7) having starting values $y_0, ..., y_{p-1}$ satisfying

$$\lim_{h \to 0} y_i = b_0, \quad i = 0, 1, 2..., p - 1.$$

Stability and consistency can be defined as follows (see e.g. [113]):

Definition 1.1.25. 1. A linear multistep method is stable, if and only if the corresponding convolution weights ω_m are bounded.

2. A linear multistep method is consistent of order p, if the following statement holds:

$$h\omega(e^{-h}) = 1 + O(h^p).$$

Now, we give two examples of a linear multistep methods, on the one hand the so called Adams method and on the other hand the backward difference formula. For both we will develop a fractional counterpart later on.

Example 1.1.26. (Adams-type) There exist two important types of Adams methods, the explicit type (Adams-Bashforth) and the implicit type (Adams-Moulton). Both have the same first characteristic polynomial, namely

$$\rho(\zeta) = \zeta^{p+1} - \zeta^p$$

but different second characteristic polynomials, which lead to two different difference equations:

$$y_{m+1} = y_m + h \sum_{k=0}^{p} \gamma_k f(t_{m-k}, y_{m-k}) \quad \text{(Adams-Bashforth)}$$

$$y_{m+1} = y_m + h \sum_{k=-1}^{p} \gamma_k f(t_{m-k}, y_{m-k}) \quad \text{(Adams-Moulton)}$$

The coefficients γ_k of the second characteristic polynomial are usually chosen to maximize the accuracy. This can e.g. be done by the solution of the ordinary differential equation $y' = f(t, y(t))$ by integration, leads to the following discretized formula

$$y(t_{m+1}) = y(t_m) + \int_{t_m}^{t_{m+1}} f(s, y(s))ds = y(t_m) + \int_{t_m}^{t_{m+1}} F(s)ds.$$

The unknown function $F(s)$ is then replaced by its polynomial interpolation at the points $t_{m-p}, ..., t_m$ (Adams-Bashforth) or $t_{m-p}, ..., t_{m+1}$ (Adams-Moulton). Then the interpolating polynomial is readily integrated to obtain the Adams-type scheme.

Example 1.1.27. (Backward difference formula) Instead of interpolation of the unknown function under the integral as in the case of the Adams-type methods we could just as easily interpolate the function $y'(t)$ on the left hand side of the ODE $y'(t) = f(t, y(t))$, then differentiate it to match the problem and thus obtain the multistep method. This approach leads to a multistep method having the general form

$$\sum_{k=-1}^{p} \beta_k y_{m-k} = hf(t_{m+1}, y_{m+1})$$

where the "convolution" weights β_k can be described as the coefficients of a Maclaurin series of a corresponding generating function given by

$$\beta(\zeta) = \sum_{k=0}^{p} \beta_k \zeta^k = \sum_{k=1}^{p} \frac{1}{k}(1 - \zeta)^k. \tag{1.9}$$

1.2 Laplace transform and some special functions

Laplace transform and the special functions as Gamma, Beta, Mittag-Leffler are most frequently used in the fractional calculus and especially in solving fractional differential equations. For this reason, we give the following definitions and theorems.

1.2.1 Laplace transform

Definition 1.2.1. Let $f(t)$ be a given function in a certain function space. Then the classical integral transform is given by

$$(Kf)(t) = \int_{-\infty}^{\infty} k(t, s)f(s)ds = g(s),$$

where $k(t, s)$ is some given function (called the kernel of the transform) and g is the transform of the function f. The most important integral transform is the Laplace transform, where

$$k(t, s) = \begin{cases} e^{-ts} & \text{if} \quad s > 0 \\ 0 & \text{if} \quad s \leq 0. \end{cases}$$

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Remark 1.2.2. Using standard notation, we write for the Laplace transform of a function $f(t)$, $0 < t < \infty$ as

$$\mathcal{L}\{f(t); p\} = \int_0^\infty e^{-pt} f(t) dt.$$

To get the solution of a differential equations of (integer or fractional) order, essentially we should give the definition of the inverse of Laplace transform.

Definition 1.2.3. Let $f(t)$ be a given function in a certain function space. Then the inverse Laplace transform is defined as

$$\mathcal{L}^{-1}\{f(p); t\} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{pt} f(p) dp,$$

where the integration is done along the vertical line $t = c$ in the complex plane such that c is greater than the real part of all singularities of $f(p)$.

The Laplace convolution of two functions $f(t)$ and $g(t)$ is defined as follows:

Definition 1.2.4. Let $f, g \in L_1(\mathbb{R})$. The Laplace convolution of f and g is denoted by $f * g$ and defined as

$$(f * g)(t) := \int_0^t f(t-u)g(u)du, \quad t > 0.$$

The Laplace transform exhibit important feature regarding the convolution of two functions f and g:

Theorem 1.2.5. *(Convolution Theorem) Let f, g be two functions for which the Laplace transform exist. Then,*

$$\mathcal{L}(f * g)(t) = \mathcal{L}(f)(t). \, \mathcal{L}(g)(t),$$

i.e. the Laplace convolution of two functions becomes a simple product in the Laplace domain.

Some special functions, important for the fractional calculus, as Gamma, Beta and Mittag-Leffler are summarized as follow (see e.g. [80, 141, 155]):

1.2.2 Gamma and Beta functions

The Gamma function, denoted by $\Gamma(z)$, is a generalization of the factorial function $n!$, i.e. $\Gamma(n) = (n-1)!$ for $n \in \mathbb{N}$. Thus, we have the following definition.

Definition 1.2.6. For $z \in \mathbb{C} \backslash \{0, -1, -2, -3, ...\}$ Gamma function $\Gamma(z)$ is defined as

$$\Gamma(z) = \begin{cases} \int_0^\infty t^{z-1} e^{-t} dt, & \text{if} \quad Re(z) > 0 \\ \\ \Gamma(z+1)/z & \text{if} \quad Re(z) \leq 0, \quad z \neq 0, -1, -2, -3, ... \end{cases} \tag{1.10}$$

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By analytic continuation the function is extended to the whole complex plane except for the point $0, -1, -2, -3, ...$, where it has simple poles. Thus, $\Gamma : \mathbb{C}\backslash\{0, -1, -2, -3, ...\} \to \mathbb{C}$.

Theorem 1.2.7. *Some of the most important properties are (for a long list of well-known properties (see e.g. [80] p.933-938)*

1. *For* $z \in \mathbb{C}\backslash\{0, -1, -2, -3, ...\}$

$$\Gamma(z + 1) = z\Gamma(z).$$

2. *For* $z \in \mathbb{C}\backslash\{0, 1, 2, 3, ...\}$

$$\Gamma(1 - z) = -z\Gamma(-z).$$

3. *Gamma function is analytic for all* $z \in \mathbb{C}\backslash\{0, -1, -2, -3, ...\}$.

4. *Gamma function is never zero.*

5. *For half-integer arguments,* $\Gamma(n/2)$, $n \in \mathbb{N}$ *has the special form*

$$\Gamma(n/2) = \frac{(n-2)!!\sqrt{\pi}}{2^{(n-1)/2}},$$

where $n!!$ *is the double factorial:*

$$n!! = \begin{cases} n.(n-2)...5.3.1 & n > 0 \quad odd \\ n.(n-2)...6.4.2 & n > 0 \quad even \\ 1 & n = 0, -1 \end{cases}$$

The graph of the function is presented in Figure 1.1. The incomplete Gamma function will also be important; this is defined as follows:

Definition 1.2.8. We define the incomplete Gamma function, $\gamma^*(v, t)$, for $Re(v) > 0$ to be

$$\gamma^*(v, t) = \frac{1}{\Gamma(v)t^v} \int_0^t \zeta^{v-1}e^{-\zeta}d\zeta.$$

A special function, which is connected to Gamma function in a direct way, is given by the Beta function, defined as follows:

Definition 1.2.9. The Beta function is defined by the integral

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

In addition, $B(z, w)$ is used sometimes for convenience to replace a combination of Gamma function. The relation between the Gamma and Beta function ([80], p.950), as follows,

$$B(z, w) = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z + w)} \tag{1.11}$$

is used later on.

1.2.3 Mittag-Leffler function

While the Gamma function is a generalization of the factorial function, the Mittag-Leffler function is a generalization of the exponential function, first introduced as a one-parameter functionm by the series (Podlubny [141], p.16). Later, the two-parameter generalization is introduced by Agarwal (see Figure 1.2), which is of great importance for the fractional calculus. It is called two-parameter function of Mittag-Leffler type. Thus, we have

Definition 1.2.10. For $z \in \mathbb{C}$ the Mittag-Leffler function $E_\alpha(z)$ is defined by

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}, \quad \alpha > 0 \tag{1.12}$$

and the generalized Mittag-Leffler function $E_{\alpha,\beta}(z)$ by

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad \alpha, \beta > 0. \tag{1.13}$$

In the following theorem we state some of the properties of the Mittag-Leffler function

Theorem 1.2.11. *The Mittag-Leffler function possesses the following properties:*

1. *For $|z| < 1$ the generalized Mittag-Leffler function satisfies*

$$\int_0^\infty e^{-t} t^{\beta-1} E_{\alpha,\beta}(t^\alpha z) dt = \frac{1}{z-1}.$$

2. *For $|z| < 1$, the Laplace transform of the Mittag-Leffler function $E_\alpha(z^\alpha)$ is given by*

$$\int_0^\infty e^{-zt} E_\alpha(z^\alpha) dt = \frac{1}{z - z^{1-\alpha}}.$$

3. *The Mittag-Leffler function (1.12) converges for every $z \in \mathbb{C}$.*

4. *For special values α the Mittag-Leffler function is given by:*

    (a) $E_0(z) = \frac{1}{1-z}$　　　*(b) $E_1(z) = e^z$*

    (c) $E_2(z^2) = \cosh(z)$　　*(d) $E_2(-z^2) = \cos(z)$*

Figure 1.1: The Gamma function for real argument.

Figure 1.2: Examples of the two-parameter function of Mittag-Leffler type.

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Chapter 2

Introduction

Fractional calculus is a mathematical branch investigating the properties of derivatives and integrals of non-integer orders (called fractional derivatives and integrals). In particular, this discipline involves the notion and methods of solving of differential equations involving fractional derivatives of the unknown function (called fractional differential equations, for short FDEs). Many of textbooks [130, 137, 141, 155] have been published on this field dealing with various aspects in different ways. Often the easiest access to the idea of the non-integer differential and integral operators studied in the field of fractional calculus is given by Cauchy's well known repersentation of an n-fold integral as a convolution integral (see Lemma 1.1.3)

$$I_a^n f(t) = \int_a^t \int_a^{s_{n-1}} ... \int_a^{s_1} f(s) ds ds_1 ds_{n-1} = \frac{1}{(n-1)!} \int_a^t (t-s)^{n-1} f(s) ds, \ n \in \mathbb{N}, t \in \mathbb{R}_+, \ (2.1)$$

where I_a^n is the n-fold integral operator (Cauchy formula).

Remark 2.0.1. The only property of the function $f(t)$ we used during the proof of the Cauchy formula was its integrability. No other restrictions are imposed.

Now, we simply generalize the Cauchy formula (2.1), the integer n is substituted by a positive real number α and the Gamma function $\Gamma(.)$ is used instead of the factorial, i.e.

$$I_a^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-s)^{\alpha-1} f(s) ds, \ \alpha, \ t \in \mathbb{R}_+.$$

The definition of fractional integral is very straightforward and there are no complications. A more difficult question is how to define a fractional derivative.

We can give the simplest definition of fractional derivative as concatenation of integer order differentiation and fractional integration, i.e.

$$D_a^\alpha f(t) = D^n I_a^{n-\alpha} f(t) \ \ or \ \ {}^C D_a^\alpha f(t) = I_a^{n-\alpha} D^n f(t),$$

where n is the integer satisfying $\alpha \leq n < \alpha + 1$ and D^n, $n \in \mathbb{N}$, is the n-fold differential operator. The operator D_a^α is usually denoted as *Riemann-Liouville differential operator*, while the operator ${}^C D_a^\alpha$ is named *Caputo differential operator*.

Because of the integral in the definition of the fractional order derivatives, it is apparent that these derivatives are non-local operators. In other word, calculating time-fractional derivative of a function $f(t)$ at some time $t = t_1$ requires all the previous history, i.e. all $f(t)$ from $t = a$ to $t = t_1$. Thus non-integer derivatives possess a memory effect, which it shares with several materials such as viscoelastic materials. This fact is also one of the reasons for the recent interest in fractional calculus: Because of their non-local property fractional derivatives can be used to construct *simple* material models and unified principles.

The fractional calculus has various applications in the physics and engineering. The first application of a semi-derivative (derivative of order 1/2) is done by Abel in 1823 (see [130, 137]). This application of fractional calculus is in relation with the solution of the integral equation for the *tautochrone problem*. Particularly in the three decade considerable interest has been shown in this extension of calculus stimulated by its applications in sciences and engineering [89, 148]. Also several fractional viscoelastic solids and fluids such as synthetic fibers [16], polybutone [149], poly (methymethacrylate) [17], nitrile rubber [63, 119], polybutadiene [120, 138], and silicone gel [121, 169] dynamic problems of linear and nonlinear hereditary mechanics of solids [150]. Glockle and Nomeenmagher [77] studied fractional protein dynamics, Mainardi [122] studied fractional relaxation, oscillations, diffusion, and wave propagation. Glockle and Nomenmacher [78, 79] and Zhang and Shimizu [181] proposed the fractional model to describe the behavior of some viscoelastic materials. They showed that this kind of models have advantages of well-defined fractional initial value. Finally, a three-dimensional formulation of linear viscoelasticity based on fractional calculus is implemented into a general purpose finite element code. Padovan and Guo [139] studied in the detail the root Locus of the fractional differential equations for various types and various values of fractional operators. Makris and Constantinou [123] studied the fractional Maxwell model for viscoelastic fluid damper for the use of earthquake isolation devices. Koh and Kelly [93] studied base isolation dampers by using viscoelastic fluid which was modeled by fractional Kelvin-Voigt model. Baker et al [18] study a partial differential equation viscoelastic model with the fractional Kelvin-Voigt law. Sugimoto et al [159, 160, 161, 162] studied initial value problems of nonlinear Burgers equation involving fractional derivative of order 1/2. Also Al-shammary et al [8] studied a fractional model to generalization of the free electron laser equation. Makris [119] studied the three-dimensional constitutive viscoelastic laws with fractional order time derivative. Mainardi [124] intermediate model of viscoelasticity, which generalize the classical Spring-dashpot model. Mainardi [125, 126] introduce the generalized Basset force, which is expressed in terms of a fractional derivative of any order α ranging in the interval $0 < \alpha < 1$. Yurity and Marina [151] collect together separated results of research in the application of fractional derivatives and other fractional operators to problem connected with vibration and waves in solids having hereditarily elastic properties, to make critical evaluation. In biology, it has been deduced that the membranes of cells of biological organism have fractional-order electrical conductance [30] and then are classified in groups of non-integer order models. Also, it has been shown that modeling the behavior of brainstem vestibule-oculumotor neurons by fractional ordinary differential equations (FODEs) has more advantages than classical integer-order modeling.

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2.1 Fractional calculus

A very brief introduction of fractional calculus has been presented. In this section we will focus our attention on the historical development of the theory of fractional calculus.

2.1.1 The history of fractional calculus

The main objects of classical calculus are derivatives and integrals of functions. If we start with a function $f(t)$ and put its derivatives on the left-hand side and on the right-hand side we continue with integrals, we obtain a both-side infinite sequence.

$$...\frac{d^2 f(t)}{dt^2}, \ \frac{df(t)}{dt}, \ f(t), \ \int_a^t f(s)ds, \ \int_a^t \int_a^{s_1} f(s)ds \ ds_1, ...$$

Fractional calculus tries to interpolate this sequence so this operation unifies the classical derivatives and integrals and generalizes them for arbitrary order. Most authors on this topic will cite a particular date as the birthday of so called "Fractional Calculus" [61, 127, 168]. In a letter [140] from Leibniz to L'Hospital dated 3.8.1695, we can find the earliest remarks on the meaning of non-integer derivatives, especially the case 1/2. In this letter Leibniz's response: "An apparent paradox, from which one day useful consequences will be drawn". In these words fractional calculus was born. Following L'Hopital's and Liebniz's first inquisition, fractional calculus was primarily a study reserved for the best minds in mathematics. Consequently, a lot of contributions to the theory of fractional calculus up to the middle of the 20-th century, of famous mathematicians are known: Laplace (1812), Fourier (1822), Abel (1823-1826), Liouville (1832-1837), Riemann (1847), Grünwald (1867-1872), Letnikov (1868-1872), Heaviside (1892-1912), Weyl (1917), Erdèlyi (1939-1965) and many others (see [73]). However, this topic is a matter of particular interest just the last thirty years. For the first specialized conference on fractional calculus and its applications has been organized by B. Ross in June 1974 at the University of New Haven, USA. For the first monograph, the merit is ascribed to K.B. Oldham and J. Spanier [137], who, after a joint collaboration began in 1968, published a book devoted to fractional calculus in 1974. In 1987, the huge book by Samko, Kilbas and Marichev, referred to now as "encyclopedia" of fractional calculus, Miller and Ross ([130], 1993), and Podlubny ([141], 1999), ect.

We now consider different definitions of fractional calculus of many famous mathematicians:

- **L. Euler (1730):**
  Euler generalized the formula

$$\frac{d^n t^m}{dt^n} = m(m-1)...(m-n+1)t^{m-n},$$

  by using of the following property of Gamma function (see Theorem 1.2.7),

$$\Gamma(m+1) = m(m-1)...(m-n+1)\Gamma(m-n+1),$$

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to obtain

$$\frac{d^n t^m}{dt^n} = \frac{\Gamma(m+1)}{\Gamma(m-n+1)} t^{m-n};$$

- **J.B.J. Fourier (1822):**
  By means of integral representation

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(z)dz \int_{-\infty}^{\infty} \cos(pt - pz)dp,$$

he wrote

$$\frac{d^n f(t)}{dt^n} = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(z)dz \int_{-\infty}^{\infty} \cos(pt - pz + n\frac{\pi}{2})dp.$$

- **N.H. Abel (1823):**
  Niels Henrik Abel used the new mathematical tool (i.e. fractional operator) to solve an integral equation arising in the *tautochrone problem* [1, 2]. Such that, he considered the integral representation $\int_0^t \frac{s'(\xi)d\xi}{(t-\xi)^\alpha} = \Psi(t)$ for arbitrary α and then wrote

$$s(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d^{-\alpha}\Psi(t)}{dt^{-\alpha}}.$$

- **J. Liouville (1832):**
  After that Abel's application for fractional operator, the first broad study of fractional calculus were carried out in a series of papers [101, 102, 103, 104, 105, 106, 107, 108] by J. Liouville. In [103] Liouville developed two different definitions of fractional derivatives:

  1. The first definition, according to exponential representation of a function

  $$f(t) = \sum_{k=0}^{\infty} c_k \exp(a_k t).$$

  He obtained by extending the known integer order derivatives $D^n e^{at} = a^n e^{at}$ to the fractional case (typically replacing $n \in \mathbb{N}$ with $\alpha \in \mathbb{C}$)

  $$D^\alpha f(t) = \sum_{k=0}^{\infty} c_k a_k^\alpha \exp(a_k t). \tag{2.2}$$

  By this definition we restrict ourselves for choice α in order to the series (2.2) be convergent.

  2. In [103] the second definition developed and it does not have such a restriction on the choice of α, but the definition is restricted on the functions of the type $f(t) = \frac{1}{t^a}$, with an arbitrary parameter a, such that

  $$D^\alpha f(t) = \frac{(-1)^\alpha \Gamma(a+\alpha)}{\Gamma(a)} t^{-a-\alpha}.$$

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- **B. Riemann (1847):**
  In 1847 Riemann worked on a paper where, searching for a generalization of a Taylor series, he deduced the definition of fractional integral of order α

  $$D^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_c^t (t-s)^{\alpha-1} f(s) \, ds + \psi(t), \tag{2.3}$$

  where $f(x)$ be a given function. We can note that equation(2.3) with lower limit $c = 0$ and without a complementary function $\psi(t)$ is the most common definition of fractional integration today, called *Riemann-Liouville fractional integral.*

- **N.Ya. Sonin (1869), A. V. Letnikov (1872), H. Laurent (1884), P.A. Nekrassov (1888):**
  In 1869 Sonin [158] wrote a paper, where he used Cauchy's integral formula as a starting point to reach differentiation with arbitrary index. Letnikov extended the idea of Sonin a short time later in 1872 in his paper [98]. Therefore, they considered the following Cauchy integral formula

  $$f^{(n)}(z) = \frac{n!}{2\pi i} \int_{\mathcal{C}} \frac{f(s)}{(s-z)^{n+1}} ds,$$

  and substituted n by α to obtain

  $$D^{\alpha} f(z) = \frac{\Gamma(\alpha+1)}{2\pi i} \int_c^{t^+} \frac{f(s)}{(s-z)^{\alpha+1}} ds,$$

  In the end it was the work of Laurent [96], who used a contour given as an open circuit (today known as Laurent loop) instead of a closed circuit used by Sonin and Letnikov and thus produced today's definition of the Riemann-Liouville fractional integral:

  $$_cD_t^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_c^t (t-s)^{\alpha-1} f(s) ds, \quad Re(\alpha) > 0,$$

  by standard contour integration methods.

- **Grünwald-Letnikov 'differintegral':**
  Grünwald-Letnikov definition of differintegral starts from classical definitions of derivatives and integrals based on infinitesimal division and limit. The disadvantages of this approach are its technical difficulty of the computations and the proofs and large restrictions on functions. Grünwald and Letnikov obtained

  $$^{GL}D_t^{\alpha} f(t) = \lim_{h \longrightarrow 0} h^{-\alpha} \sum_{k=0}^{\left[\frac{t}{h}\right]} (-1)^k \binom{\alpha}{k} f(t-kh), \quad \alpha > 0,$$

  where $[t]$ means the integer part of t, h is the step-size and $\binom{\alpha}{k}$ is the generalized binomial coefficient.

- **Riemann-Liouville definition:**
  Fortunately there is other, more elegant approach like the Riemann-Liouville definition which includes the results of the Grünwald-Letnikov as a special case.

$$ {}_aD_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_a^t \frac{f(s)ds}{(t-s)^{\alpha-n+1}}, \quad (n-1 < \alpha \le n), n \in \mathbb{N}. $$

  The Riemann-Liouville derivative has certain disadvantages when trying to model real-world phenomena with fractional differential equations. Therefore, we shall introduce a modified fractional differential operator proposed by Caputo [46, 51, 137].

- **M. Caputo (1967):**
  This is the popular definition of fractional calculus,

$$ {}_a^C D_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \int_a^t \frac{f^{(n)}(s)ds}{(t-s)^{\alpha-n+1}}, \quad (n-1 < \alpha \le n), n \in \mathbb{N}. $$

2.1.2 Merit of using fractional-order

Differential equations of fractional order have been the focus of many studies due to their frequent appearance in various applications in fluid mechanics, viscoelasticity, biology, physics and engineering. For example, many real dynamic systems are better characterized using a non-integer order dynamic model based on fractional differentiation or integration. The most important advantage of using FDEs in these and other applications is their non-local property. It is well knwon that the integer order differential operator is a local operator but the fractional order differential operator is non-local. This means that the next state of a system depend not only upon its current state but also upon all historical states. This is more realistic, and the results derived of the fractional systems are more general nature. However, the fundamental solutions of these equations still exhibit useful scaling properties that make them attractive for applications [141]. We would like to put your attention that time fractional derivatives change also the solutions we usually get in standard integer form. The concept of fractional or non-integer order derivation and integration can be traced back to the genesis of integer order calculus itself. Most of the mathematical theory applicable to the study of non-integer order calculus was developed through the end of 19-th century. However it is in the past hundred years that the most intriguing leaps in engineering and scientific application have been found. The calculation technique has in some cases had to change to meet the requirement of physical reality. The derivatives are understood in the Caputo sense. The general response expression contains a parameter describing the order of the fractional derivative that can be varied to obtain various responses. One of the basic reasons of using fractional order differential equations is that [36, 109] "***Fractional order differential equations are, at least, as stable as their integer order counterpart***".

2.1.3 Physical and Geometric interpretation

In general, fractional calculus, closely related to classical calculus, is not direct generalization of classical calculus in the sense of rigorous mathematics. We well know the geometrical and physical meaning of the classical calculus (i.e. integration and differentiation). For example, the integral $A = \int_a^b f(x)dx$, from the viewpoint of geometry, it means the area of the domain $\{(x,y)|\ a \le x < b,\ 0 \le y \le f(x)\}$ presuming that $f(x) \ge 0$. From the viewpoint of physics, it implies the displacement from a to b if $f(x)$ indicates the velocity at time x. For the derivative, e.g. $f'(x)$ indicates the slope of the curve $f(x)$ at x and on the other hand, the position of a moving object can be represented as a function of time $s(t)$, then the object's velocity is the first derivative of this function (i.e. $s'(t)$), the acceleration is the second derivative $s''(t)$.

Now, for a possible interpretation of the fractional calculus. Some authors (see [133]) consider the fractional operators as linear filters and also seek the geometrical interpretation of the fractional operators in the fractal geometry, of which classical geometry is a subclass. The fractal Cantor's set and a domino ladder network (series of resistors and capacitors that can be connected in different configurations) are used as illustration. The conventional physics and geometry are restricted to rigid boundaries and integer dimensions. Functions and processes that fall between discrete dimensions cannot be described. An example of it is a Cantor's set that has a dimension between that of a line and a point. But by means of fractal geometry the properties of any system with non-integer dimension can be interpreted geometrically.

Podlubny, in [143], provides a physical interpretation of the fractional integration in terms of two different time scales, namely, the homogeneous, equably flowing scale and the inhomogeneous time scale.

Finally, in [111] the authors give possible physical and geometrical interpretation as follow: Form (2.4) the fractional integral with order α can be rewritten as

$$I_a^\alpha f(t) = \int_a^t f(\tau)dY_\alpha(\tau),$$

where

$$Y_\alpha(\tau) = \begin{cases} -\dfrac{(t-\tau)^\alpha}{\Gamma(\alpha+1)}, & \tau \in [a,t], \\ 0, & \tau < a. \end{cases}$$

This is the standard *Stieltjes integral*. $Y_\alpha(\tau)$ is a monotonously increasing function in $(-\infty, t]$. The positive number α is an index characterizing the singularity: the smaller α, the stronger singularity the integral. So $I_a^\alpha f(t)$ indicates the generalized area in the sense of length $Y_\alpha(\tau)$ (geometrical meaning) or the generalized displacement in the sense of $Y_\alpha(\tau)$ if $f(t)$ means the velocity at time t (physical meaning).

From (2.10) and (2.11) the Riemann-Liouville, Caputo derivative with order $0 < \alpha < 1$ can be written as, respectively

$$_aD_t^\alpha f(t) = \frac{d}{dt}\int_a^t f(\tau)dY_{1-\alpha}(\tau),$$

$$ {}^C_a D^\alpha_t f(t) = \int_a^t f'(\tau) dY_{1-\alpha}(\tau), $$

where

$$ Y_{1-\alpha}(\tau) = \begin{cases} -\dfrac{(t-\tau)^{1-\alpha}}{\Gamma(2-\alpha)}, & \tau \in [a,t], \\ 0, & \tau < a. \end{cases} $$

Obviously, $Y_{1-\alpha}(\tau)$ is a monotonously increasing function in $(-\infty, t]$. So ${}_a D^\alpha_t f(t)$ indicates the generalized slope in the sense of length $Y_{1-\alpha}(\tau)$ if $f(t)$ means the slope (geometrical meaning) or the generalized velocity in the sense of length $Y_{1-\alpha}(\tau)$ if $f(t)$ means the velocity (physical meaning). Also, ${}^C_a D^\alpha_t f(t)$ indicates the generalized displacement of the curve $f(t)$ in the sense of length $Y_{1-\alpha}(\tau)$ (physical meaning) if $f(t)$ means the displacement, or represents the generalized curve in the sense of length $Y_{1-\alpha}(\tau)$ if $f(t)$ is a curve (geometrical meaning).

2.1.4 Fractional integration and differentiation

As seen in the historical outline in Subsection 2.1.1 , more than one way to transfer integer-order operations to the non-integer case was developed. We will focus on the Riemann-Liouville, the Caputo operators since they are the most used ones in applications and also Grünwald-Letnikov operator. The results of this subsection are greater parts well known and can be found in various books (see e.g. [130, 137, 141, 155]). Now, Let $L_1 = L_1[a,b]$ be the class of integrable functions on the interval $[a,b]$, $0 \le a < b < \infty$ with the norm defined by:

$$ \|f(t)\| = \int_a^b |f(s)| ds, \quad t \in [a,b]. $$

Definition 2.1.1. Let $\alpha \in \mathbb{R}_+$. The operator I^α_a, defined on $L_1[a,b]$ by

$$ I^\alpha_a f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-s)^{\alpha-1} f(s) ds, \tag{2.4} $$

for $a \le t \le b$, is called the Riemann-Liouville fractional integral operator of order α. For $\alpha = 0$, we set $I^\alpha_0 := I$, the *identity operator*. When $a = 0$, the fractional integral of order $\alpha > 0$ can be considered as the *Laplace convolution* between the causal function $\phi_\alpha(t)$ and $f(t)$, i.e. (see [67])

$$ I^\alpha_0 f(t) = I^\alpha f(t) = f(t) * \phi_\alpha(t), \quad \alpha > 0 \tag{2.5} $$

where

$$ \phi_\alpha(t) = \begin{cases} \dfrac{t^{\alpha-1}}{\Gamma(\alpha)}, & \text{for} \quad t > 0, \\ \\ 0, & \text{for} \quad t \le 0. \end{cases} \tag{2.6} $$

and $\phi_\alpha(t)$ satisfies the following properties

1. $\phi_\alpha(t) * \phi_\beta(t) = \phi_{\alpha+\beta}(t), \quad \alpha + \beta > 0$ (*The composition rule*).

2. $\frac{d}{dt}\phi_\alpha(t) = \phi_{\alpha-1}(t)$.

3. $\lim_{\alpha \to 0} \phi_\alpha(t) = \phi_0(t) = \delta(t), \ \alpha > 1$

where $\delta(t)$ is dirac delta function.

If $\alpha \in \mathbb{N}$ the Riemann-Liouville fractional integral coincides with the classical integral I_a^n in equation (2.1) except that the domain has been extended from Riemann integrable to Lebesgue integrable functions. With the existence of fractional integral of Definition 2.1.1 guaranteed (see e.g. [130]), we can give the following properties (see [89, 130, 155]):

Lemma 2.1.2. *For $\alpha, \ \beta > 0$ and $f(t) \in L_1[a, b]$, we have*

$$I_a^\alpha I_a^\beta f(t) = I_a^{\alpha+\beta} f(t) = I_a^\beta I_a^\alpha f(t). \tag{2.7}$$

And,

$$(I_a^\alpha)^n f(t) = I_a^{\alpha n} f(t); \quad n = 1, 2, 3, \dots, \tag{2.8}$$

which is a well known result in the integer case.

Proof. We will prove that relations (2.7) and (2.8) holds almost everywhere. We choose $a \in \mathbb{R}$, $\alpha, \ \beta > 0$, $f(t)$ an integrable function. During the computation we use the change of order of integration and the Beta function. By definition of the fractional integral we have

$$I_a^\alpha I_a^\beta f(t) = \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^t (t-s)^{\alpha-1} \int_a^s (s-\tau)^{\beta-1} f(\tau) d\tau \ ds.$$

Since, the integrals exist, and by Fubini's theorem (Theorem 1.1.10) we may interchange the order of integration, obtaining

$$
\begin{aligned}
I_a^\alpha I_a^\beta f(t) &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^t \int_\tau^t (t-s)^{\alpha-1}(s-\tau)^{\beta-1} f(\tau) ds \ d\tau \\
&= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^t f(\tau) \int_\tau^t (t-s)^{\alpha-1}(s-\tau)^{\beta-1} ds \ d\tau.
\end{aligned}
$$

By the substitution $u = \dfrac{s-\tau}{t-\tau}$, we have

$$I_a^\alpha I_a^\beta f(t) = \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^t f(\tau)(t-\tau)^{\alpha+\beta-1} \int_0^1 (1-u)^{\alpha-1} u^{\beta-1} du \ d\tau,$$

The term $\int_0^1 (1-u)^{\alpha-1} u^{\beta-1} du$ is the Beta function, and thus

$$I_a^\alpha I_a^\beta f(t) = \frac{1}{\Gamma(\alpha+\beta)} \int_a^t (t-s)^{\alpha+\beta-1} f(\tau) d\tau = I_a^{\alpha+\beta} f(t).$$

holds almost everywhere on $[a, b]$. Similarly we can obtain

$$I_a^\beta I_a^\alpha f(t) = I_a^{\alpha+\beta} f(t).$$

So we just proved that fractional integrals are commutative (exactly the same result we have in classical calculus). Consequently, we have

$$
\begin{aligned}
(I_a^\alpha)^n f(t) &= I_a^\alpha I_a^\alpha I_a^\alpha ... I_a^\alpha f(t) \\
&= I_a^{\alpha n} f(t).
\end{aligned}
$$

$\square$

Lemma 2.1.3. *Let I_a^α be defined in L_1, then as $\alpha \to n$ we have*

$$I_a^\alpha f(t) \to I_a^n f(t), \text{uniformly in } L_1, \quad n = 1, 2, ... \ ,$$

where $I_a f(t)$ defined by equation (1.1)

Proof. Let $f(t) \in L_1$, then from the inequality

$$|I_a^\alpha f(t) - I_a^n f(t)| \le \int_a^t \left| \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} - \frac{(t-s)^{n-1}}{\Gamma(n)} \right| |f(s)| ds.$$

But since $\frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} \to \frac{(t-s)^{n-1}}{\Gamma(n)}$ as $\alpha \to n$, $n = 1, 2, ... \ $, then we get $I_a^\alpha f(t) \to I_a^n f(t)$. $\square$

Theorem 2.1.4. *If $f(t)$ is continuous on $[a, b]$, then*

$$\lim_{\alpha \to 0} I_a^\alpha f(t) = f(t).$$

Proof. If $f(t)$ has continuous derivative for $t \ge a$. In such case, integration by parts gives

$$
\begin{aligned}
I_a^\alpha f(t) &= \int_a^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} f(s) ds \\
&= \frac{(t-a)^\alpha}{\Gamma(\alpha+1)} f(a) + \int_a^t \frac{(t-s)^\alpha}{\Gamma(\alpha+1)} f'(s) ds,
\end{aligned}
$$

and we have

$$
\begin{aligned}
\lim_{\alpha \to 0} I_a^\alpha f(t) &= f(a) + \int_a^t f'(s) ds \\
&= f(a) + f(t) - f(a) = f(t).
\end{aligned}
$$

Now, if $f(t)$ is only continuous for $t \ge a$, then let $I_a^\alpha f(t)$ be written in the following form,

$$
\begin{aligned}
I_a^\alpha f(t) &= \int_a^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} f(s) ds \\
&= \int_a^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} (f(s) - f(t)) ds + \frac{f(t)}{\Gamma(\alpha)} \int_a^t (t-s)^{\alpha-1} ds
\end{aligned}
$$

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$$I_a^\alpha f(t) = \int_a^{t-\delta} \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds + f(t)\frac{(t-s)^\alpha}{\Gamma(\alpha+1)} + \int_{t-\delta}^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds. \quad (2.9)$$

Let us consider, the second integration in the right hand side of equation (2.9), for every $\delta > 0$ there exist $\epsilon > 0$, such that $|f(s) - f(t)| < \epsilon$, then we have the following estimate of the integral

$$\left| \int_{t-\delta}^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds \right| \quad < \quad \frac{\epsilon}{\Gamma(\alpha)}\int_{t-\delta}^t (t-s)^{\alpha-1}ds$$

$$< \quad \frac{\epsilon\delta^\alpha}{\Gamma(\alpha+1)}.$$

And taking into account that $\epsilon \to 0$ as $\delta \to 0$, we obtain for all $\alpha > 0$

$$\lim_{\delta \to 0} \left| \int_{t-\delta}^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds \right| = 0,$$

taking an arbitrary $\epsilon > 0$ and choose δ such

$$\left| \int_{t-\delta}^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds \right| < \epsilon, \quad \forall \alpha \geq 0.$$

For fixed δ we obtain the following estimate of the first integral in the right hand side of equation (2.9)

$$\left| \int_a^{t-\delta} \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds \right| \quad \leq \quad \frac{\epsilon}{\Gamma(\alpha)}\int_a^{t-\delta} (t-s)^{\alpha-1}ds$$

$$\leq \quad \frac{\epsilon}{\Gamma(\alpha+1)}((t-a)^\alpha - \delta^\alpha),$$

then, it follow that for fixed $\delta > 0$

$$\lim_{\alpha \to 0} \left| \int_a^{t-\delta} \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds \right| = 0.$$

Considering

$$|I_a^\alpha f(t) - f(t)| \quad = \quad \left| \int_a^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds \right| + \left| \int_a^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}f(t)ds - f(t) \right|$$

$$\leq \quad \left| \int_a^{t-\delta} \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds \right| + \left| \int_{t-\delta}^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}(f(s)-f(t))ds \right|$$

$$+ \quad |f(t)| \, |\frac{(t-s)^\alpha}{\Gamma(\alpha+1)} - 1|,$$

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and taking into account the limits and the estimates we obtain

$$\lim_{\alpha \to 0} \sup |I_a^\alpha f(t) - f(t)| \leq \epsilon,$$

where ϵ can be chosen as small as we wish therefore

$$\lim_{\alpha \to 0} \sup |I_a^\alpha f(t) - f(t)| = 0,$$

and then

$$I_a^\alpha f(t) \to f(t) \quad \text{as} \quad \alpha \to 0.$$

$\square$

We now consider the following examples for fractional integration,

Example 2.1.5. For $\alpha > 0$ and $t > 0$, we have

$$I^\alpha t^\lambda = \frac{\Gamma(1 + \lambda)}{\Gamma(\lambda + \alpha + 1)} t^{\lambda + \alpha}, \quad \lambda > -1.$$

In particular, if $\lambda = 0$, then the fractional integral of a constant k of order α is

$$I^\alpha k = \frac{k}{\Gamma(\alpha + 1)} t^\alpha.$$

Example 2.1.6. Let $f(t) = (t - a)^\lambda$ for some $\lambda > -1$ and $\alpha > 0$. Then,

$$I_a^\alpha f(t) = \frac{\Gamma(\lambda + 1)}{\Gamma(\lambda + \alpha + 1)} (t - a)^{\alpha + \lambda}.$$

Example 2.1.7. Let $\alpha > 0$, $\lambda > -1$, and $t > 0$ then we have

$$I^\alpha (t^\lambda + 1) = \frac{\Gamma(\lambda + 1)}{\Gamma(\lambda + \alpha + 1)} t^{\lambda + \alpha} + \frac{t^\alpha}{\Gamma(\alpha + 1)}.$$

Example 2.1.8. Let $f(t) = e^{at}$, where a is constant, e^{at} is of class C, and by Definition 2.1.1, we have

$$I^\alpha e^{at} = \frac{1}{\Gamma(\alpha)} \int_0^t (t - s)^{\alpha - 1} e^{as} ds, \quad \alpha > 0.$$

If we make the change of variable $x = t - s$, then we have

$$I^\alpha e^{at} = \frac{e^{at}}{\Gamma(\alpha)} \int_0^t x^{\alpha - 1} e^{-ax} dx, \quad \alpha > 0,$$

the above relation becomes to

$$I^\alpha e^{at} = t^\alpha e^{at} \gamma^*(\alpha, at),$$

where γ^* is incomplete Gamma function (see Definition 1.2.8), the right-hand side of above equation is the fractional integral of an exponential function and we shall call it $E_t(\alpha, a)$, then $I^\alpha e^{at} = E_t(\alpha, a)$.

Until now we only considered the Riemann-Liouville integral operator. For a classical case we have the identity (1.2) (under certain conditions) and we can now motivate the definition of the fractional differential operator by generalizing this identity to non-integer order. There are different definitions for fractional derivatives, which do not coincide in general.

Definition 2.1.9. Suppose that $\alpha > 0$, $t > a$, $\alpha, a, t \in \mathbb{R}$. Then (see [130, 142])

$$
{}_aD_t^\alpha f(t) := \begin{cases} \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_a^t \frac{f(s)}{(t-s)^{\alpha-n+1}} ds = \frac{d^n}{dt^n} I_a^{n-\alpha} f(t), & n-1 < \alpha < n \in \mathbb{N}, \\ \\ \frac{d^n}{dt^n} f(t), & \alpha = n \in \mathbb{N}, \end{cases} \tag{2.10}
$$

is called the Riemann-Liouville fractional derivative or the Riemann-Liouville fractional differential operator of order α. We note that this operator is the left-inverse operator of the fractional integral (2.4) (see [73]), i.e., $D^\alpha I^\alpha f(t) = f(t)$.

In 1967 a paper [25] by the Italian mathematician M. Caputo was published, where a new definition of a fractional derivative was used. Now, we state the definition and some properties of Caputo fractional derivative.

Definition 2.1.10. Suppose that $\alpha > 0$, $t > a$, $\alpha, a, t \in \mathbb{R}$. The fractional operator

$$
{}_a^CD_t^\alpha f(t) := \begin{cases} \frac{1}{\Gamma(n-\alpha)} \int_a^t \frac{f^{(n)}(s)}{(t-s)^{\alpha-n+1}} ds = I_a^{n-\alpha} D^n f(t), & n-1 < \alpha < n \in \mathbb{N}, \\ \\ \frac{d^n}{dt^n} f(t), & \alpha = n \in \mathbb{N}, \end{cases} \tag{2.11}
$$

is called the Caputo fractional derivative or Caputo fractional differential operator of order α.

These definitions are more convenient in many applications in physics, engineering and applied science. But, in Caputo definition we find a link between what is possible and what is practical.

Remark 2.1.11. Here the symbols ${}_aD_t^\alpha f(t)$ and ${}_a^CD_t^\alpha f(t)$ are used for the Riemann-Liouville and Caputo fractional derivatives respectively (see [141]), a and t are called terminals (lower and upper correspondingly), if $a = 0$ then the symbols $D^\alpha f(t)$ and ${}^CD^\alpha f(t)$ are adopted.

Lemma 2.1.12. *Let $f(t)$ be an absolutely continuous function on $[a,b]$ and $\alpha > 0$. If $f(a) = 0$, then*

$$
\frac{d}{dt} I_a^\alpha f(t) = I_a^\alpha \frac{d}{dt} f(t).
$$

Proof.

$$
\begin{aligned}
I_a^\alpha f(t) &= \int_a^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} f(s) ds \\
&= -f(s) \frac{(t-s)^\alpha}{\Gamma(\alpha+1)} \Big|_a^t + \int_a^t \frac{(t-s)^\alpha}{\Gamma(\alpha+1)} f'(s) ds \\
&= f(a) \frac{(t-a)^\alpha}{\Gamma(\alpha+1)} + I_a^{1+\alpha} f'(t).
\end{aligned}
$$

Then,

$$\frac{d}{dt} I_a^\alpha f(t) = f(a) \frac{(t-a)^{\alpha-1}}{\Gamma(\alpha)} + I_a^\alpha f'(t),$$

If $f(a) = 0$, then

$$\frac{d}{dt} I_a^\alpha f(t) = I_a^\alpha \frac{d}{dt} f(t).$$

$\square$

Theorem 2.1.13. (**i**) *Let* α, $\beta \in (0,1)$ *and* $f(t)$ *is absolutely continuous function on* $[a,b]$. *If* $f'(t)$ *is bounded and* $\alpha + \beta \in (0,1)$, *then*

$$^C_a D_t^\alpha \ {}^C_a D_t^\beta f(t) = \ {}^C_a D_t^{\alpha+\beta} f(t) = \ {}^C_a D_t^\beta \ {}^C_a D_t^\alpha f(t).$$

(**ii**) *Let* $\alpha \in (0,1)$. *If* $f(t)$ *is absolutely continuous function on* $[a,b]$, *then*

(a)

$$I_a^\alpha \ {}^C_a D_t^\alpha f(t) = f(t) - f(a).$$

(b)

$$^C_a D_t^\alpha I_a^\alpha f(t) = f(t).$$

Proof. (**i**) We can write

$$^C_a D_t^\alpha \ {}^C_a D_t^\beta f(t) = I_a^{1-\alpha} D I_a^{1-\beta} D f(t),$$

since $f'(t)$ is bounded, then $I_a^{1-\beta} D f(t)|_{t=a} = 0$ and hence

$$\begin{aligned}
^C_a D_t^\alpha \ {}^C_a D_t^\beta f(t) &= D I_a^{2-(\alpha+\beta)} D f(t) \\
&= D I_a I_a^{1-(\alpha+\beta)} D f(t) \\
&= I_a^{1-(\alpha+\beta)} D f(t) = \ {}^C_a D_t^{\alpha+\beta} f(t).
\end{aligned}$$

Similarly, we can prove that

$$^C_a D_t^\beta \ {}^C_a D_t^\alpha f(t) = \ {}^C_a D_t^{\alpha+\beta} f(t).$$

(**ii**) (**a**) For this part, we have

$$\begin{aligned}
I_a^\alpha \ {}^C_a D_t^\alpha f(t) &= I_a^\alpha I_a^{1-\alpha} D f(t) \\
&= I_a D f(t) = f(t) - f(a).
\end{aligned}$$

(**b**) Since $f(t)$ is bounded and measurable, then $I_a^\alpha f(t)|_{t=a} = 0$, so

$$\begin{aligned}
^C_a D_t^\alpha I_a^\alpha f(t) &= I_a^{1-\alpha} D I_a^\alpha f(t) \\
&= I_a^{1-\alpha} I_a^\alpha D f(t) = I_a D f(t) = f(t).
\end{aligned}$$

$\square$

Lemma 2.1.14. *Let* $n - 1 < \alpha < n$, $n \in \mathbb{N}$, $\alpha \in \mathbb{R}$ *and* $f(t)$ *be such that* ${}^C D^\alpha f(t)$ *exists. Then the following properties for the Caputo operator hold*

$$
\begin{aligned}
\lim_{\alpha \to n} {}^C D_t^\alpha f(t) &= f^{(n)}(t), \\
\lim_{\alpha \to n-1} {}^C D_t^\alpha f(t) &= f^{(n-1)}(t) - f^{(n-1)}(0).
\end{aligned}
$$

Proof. The proof uses integration by parts (see [141], p.79).

$$
\begin{aligned}
{}^C D_t^\alpha f(t) &= \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{f^{(n)}(s)}{(t-s)^{\alpha-n+1}} ds \\
&= \frac{1}{\Gamma(n-\alpha)} \left(-f^{(n)}(s) \frac{(t-s)^{n-\alpha}}{n-\alpha} \Big|_0^t + \int_0^t f^{(n+1)}(s) \frac{(t-s)^{n-\alpha}}{n-\alpha} ds \right) \\
&= \frac{1}{\Gamma(n-\alpha+1)} \left(f^{(n)}(0) t^{n-\alpha} + \int_0^t f^{(n+1)}(s)(t-s)^{n-\alpha} ds \right).
\end{aligned}
$$

Now, by taking the limit for $\alpha \to n$ and $\alpha \to n-1$, respectively, it follows

$$
\lim_{\alpha \to n} {}^C D_t^\alpha f(t) = (f^{(n)}(0) + f^{(n)}(s))|_{s=0}^t = f^{(n)}(t)
$$

and

$$
\lim_{\alpha \to n-1} {}^C D_t^\alpha f(t) = (f^{(n)}(0) t + f^{(n)}(s)(t-s))|_{s=0}^t + \int_0^t f^{(n)}(s) ds
$$

$$
= f^{(n-1)}(s)|_{s=0}^t = f^{(n-1)}(t) - f^{(n-1)}(0).
$$

For the Riemann-Liouville fractional derivative the corresponding property reads

$$
\lim_{\alpha \to n} D_t^\alpha f(t) = f^{(n)}(t),
$$

$$
\lim_{\alpha \to n-1} D_t^\alpha f(t) = f^{(n-1)}(t).
$$

$\square$

Now the following theorem shows the relation between the two definitions [73].

Theorem 2.1.15. *Let* $t > 0$, $\alpha \in \mathbb{R}$, $n - 1 < \alpha < n \in \mathbb{N}$. *Then the following relation between the Riemann-Liouville (2.10) and the Caputo (2.11) derivatives holds*

$$
{}^C D_t^\alpha f(t) = D_t^\alpha f(t) - \sum_{k=0}^{n-1} \frac{t^{k-\alpha}}{\Gamma(k+1-\alpha)} f^{(k)}(0).
$$

Proof. The well-known Taylor series expansion about the point 0 reads (see Theorem 1.1.8)

$$f(t) = \sum_{k=0}^{n-1} \frac{t^k}{\Gamma(k+1)} f^{(k)}(0) + I^n f^{(n)}(t).$$

Now, by the Riemann-Liouville fractional derivative we obtain

$$\begin{aligned}
D_t^\alpha f(t) &= D_t^\alpha \left(\sum_{k=0}^{n-1} \frac{t^k}{\Gamma(k+1)} f^{(k)}(0) + I^n f^{(n)}(t) \right) \\
&= \sum_{k=0}^{n-1} \frac{D_t^\alpha t^k}{\Gamma(k+1)} f^{(k)}(0) + D_t^\alpha I^n f^{(n)}(t) \\
&= \sum_{k=0}^{n-1} \frac{t^{k-\alpha}}{\Gamma(k-\alpha+1)} f^{(k)}(0) + I^{n-\alpha} f^{(n)}(t) \\
&= \sum_{k=0}^{n-1} \frac{t^{k-\alpha}}{\Gamma(k+1-\alpha)} f^{(k)}(0) + {}^C D_t^\alpha f(t)
\end{aligned}$$

This means that,

$${}^C D_t^\alpha f(t) = D_t^\alpha f(t) - \sum_{k=0}^{n-1} \frac{t^{k-\alpha}}{\Gamma(k+1-\alpha)} f^{(k)}(0), \tag{2.12}$$

this formula implies that the two definitions coincides if and only if $f(t)$ together with its first $n-1$ derivatives vanish at $t=0$. □

Corollary 2.1.16. *The following relation between the Riemann-Liouville and Caputo fractional derivatives holds*

$${}^C D^\alpha f(t) = D^\alpha \left(f(t) - \sum_{k=0}^{n-1} \frac{t^k}{k!} f^{(k)}(0) \right).$$

Proof. This formula is proved (see [73]) using relation (2.12), i.e.,

$$\begin{aligned}
{}^C D^\alpha f(t) &= D^\alpha f(t) - \sum_{k=0}^{n-1} \frac{t^{k-\alpha}}{\Gamma(k+1-\alpha)} f^{(k)}(0) \\
&= D^\alpha f(t) - \sum_{k=0}^{n-1} \frac{D^\alpha t^k}{\Gamma(k+1)} f^{(k)}(0) \\
&= D^\alpha \left(f(t) - \sum_{k=0}^{n-1} \frac{t^k}{k!} f^{(k)}(0) \right).
\end{aligned}$$

□

The following table shows the main properties for D^α and ${}^C D^\alpha$ operators.

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Property	Riemann-Liouville	Caputo
Representation	$D^\alpha f(t) = D^n I^{n-\alpha} f(t)$	$^C D^\alpha f(t) = I^{n-\alpha} D^n f(t)$
Interpolation	$\lim_{\alpha \to n} D^\alpha f(t) = f^{(n)}(t)$ $\lim_{\alpha \to n-1} D^\alpha f(t) = f^{(n-1)}(t)$	$\lim_{\alpha \to n} {}^C D^\alpha f(t) = f^{(n)}(t)$ $\lim_{\alpha \to n-1} {}^C D^\alpha f(t) = f^{(n-1)}(t) - f^{(n-1)}(0)$
Linearity	$D^\alpha(\lambda f(t) + g(t)) = \lambda D^\alpha f(t) + D^\alpha g(t)$	$^C D^\alpha(\lambda f(t) + g(t)) = \lambda \, {}^C D^\alpha f(t) + {}^C D^\alpha g(t)$
Non-commutation	$D^m D^\alpha f(t) = D^{\alpha+m} f(t) \neq D^\alpha D^m f(t)$	$^C D^\alpha D^m f(t) = {}^C D^{\alpha+m} f(t) \neq D^m \, {}^C D^\alpha f(t)$
Laplace transform	$\mathscr{L}\{D^\alpha f(t); s\} = s^\alpha F(s) - \sum_{k=0}^{n-1} s^k [D^{\alpha-k-1} f(t)]_{t=0}$	$\mathscr{L}\{ {}^C D^\alpha f(t); s\} = s^\alpha F(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} f^{(k)}(0)$
Leibniz rule	$D^\alpha(f(t)g(t)) = \sum_{k=0}^{\infty} \binom{\alpha}{k} (D^{\alpha-k} f(t)) g^{(k)}(t)$	$^C D^\alpha(f(t)g(t)) = \sum_{k=0}^{\infty} \binom{\alpha}{k} (D^{\alpha-k} f(t)) g^{(k)}(t)$ $- \sum_{k=0}^{n-1} \frac{t^{k-\alpha}}{\Gamma(k+1-\alpha)} ((f(t)g(t))^{(k)}(0))$
$f(t) = c = $ constant	$D^\alpha c = \frac{c}{\Gamma(1-\alpha)} t^{-\alpha} \neq 0, \quad c = \mathrm{const}$	$^C D^\alpha c = 0, \quad c = \mathrm{const}$

Table 2.1: Comparison between Riemann-Liouville and Caputo fractional derivatives.

We now consider the following examples for fractional derivative (Caputo's sense),

Example 2.1.17. Let $\alpha \in (0,1]$ and $\lambda > 0$, then we have

$$^{C}D_a^\alpha(t-a)^\lambda = \frac{\Gamma(\lambda+1)}{\Gamma(1+\lambda-\alpha)}(t-a)^{\lambda-\alpha},$$

also,

$$\lim_{\alpha\to 1} {}^{C}D_a^\alpha(t-a)^\lambda = \lambda(t-a)^{\lambda-1}, \quad \text{and} \quad \lim_{\alpha\to 0} {}^{C}D_a^\alpha(t-a)^\lambda = (t-a)^\lambda.$$

Example 2.1.18. Let $\alpha \in (0,1]$ and $\lambda > -1$, then we have

$$
\begin{aligned}
^{C}D^\alpha(1+t^\lambda) &= I^{1-\alpha}(\lambda\,t^{\lambda-1}) = \lambda I^{1-\alpha}t^{\lambda-1} \\[2mm]
&= \lambda\frac{\Gamma(\lambda)}{\Gamma(\lambda-\alpha+1)}t^{\lambda-\alpha} = \frac{\Gamma(\lambda+1)}{\Gamma(\lambda-\alpha+1)}t^{\lambda-\alpha}.
\end{aligned}
$$

And,

$$
\begin{aligned}
D^\alpha(1+t^\lambda) &= DI^{1-\alpha}(1+t^\lambda) \\[2mm]
&= D\left(\frac{t^{1-\alpha}}{\Gamma(2-\alpha)} + \frac{\Gamma(\lambda+1)}{\Gamma(\lambda-\alpha+2)}t^{\lambda-\alpha+1}\right) \\[2mm]
&= \frac{(1-\alpha)t^{-\alpha}}{\Gamma(2-\alpha)} + \frac{(\lambda-\alpha+1)\Gamma(\lambda+1)}{\Gamma(\lambda-\alpha+2)}t^{\lambda-\alpha} \\[2mm]
&= \frac{t^{-\alpha}}{\Gamma(1-\alpha)} + \frac{\Gamma(\lambda+1)}{\Gamma(\lambda-\alpha+1)}t^{\lambda-\alpha},
\end{aligned}
$$

which verifies that $D^\alpha f(t) \neq {}^{C}D^\alpha f(t)$.

Nearly simultaneously with the development of the Riemann-Liouville definition of fractional integration and differentiation another definition for a non-integer derivative was developed independently by Grünwald and Letnikov. We start from the fundamental definition a derivative, shown in (2.13)

$$f'(t) = \lim_{h\to 0} \frac{f(t+h) - f(t)}{h}, \tag{2.13}$$

for the nth derivative, we can introduce the operator D^n to represent the n-repetitions of the derivative.

$$D^n f(t) = \lim_{h\to 0} \frac{1}{h^n} \sum_{k=0}^{n} (-1)^k \binom{n}{k} f(t-kh).$$

This expression can be generalized for non-integer values for n with $\alpha \in \mathbb{R}$ provided that the binomial coefficient be understood as using the Gamma function in place of the standard factorial. Also, the upper limit of the summation (no longer the integer, n) goes to infinity as $\frac{t-a}{h}$ (where t and a are the upper and lower limits of differentiation, respectively). Now, we can state the definition of Grünwald-Letnikov fractional derivative.

Definition 2.1.19. Let $\alpha \in \mathbb{R}_+$. The operator $^{GL}D_a^\alpha$, defined by

$$^{GL}D_a^\alpha f(t) = \lim_{\substack{h \to 0 \\ mh=t-a}} \frac{1}{h^\alpha} \sum_{k=0}^{m} (-1)^k \binom{\alpha}{k} f(t-kh), \quad \alpha > 0 \qquad (2.14)$$

for $a \leq t \leq b$, is called the Grünwald-Letnikov fractional derivative of order α.

The definition holds for arbitrary functions $f(t)$, but the convergence of the infinite sum cannot be ensured for all functions. To define Grünwald-Letnikov fractional integral of order α, we can rewrite (2.14) for $-\alpha$, i.e.

$$^{GL}I_a^\alpha f(t) = \lim_{\substack{h \to 0 \\ mh=t-a}} h^\alpha \sum_{k=0}^{m} (-1)^k \binom{-\alpha}{k} f(t-kh) = \lim_{\substack{h \to 0 \\ mh=t-a}} \frac{h^\alpha}{\Gamma(\alpha)} \sum_{k=0}^{m} \frac{\Gamma(k+\alpha)}{\Gamma(k+1)} f(t-kh), \quad \alpha > 0.$$
$$(2.15)$$

Thus, the Grünwald-Letnikov definition of differintegral starts from classical definition of derivative and integral based on infinitesimal division and limit. The advantage of this approach is very easily utilized for numerical evaluation to differential equations of fractional order.

We now state the following important results, which will give us the connection between the Grünwald-Letnikov derivative and the two earlier defined fractional derivatives, namely the Riemann-Liouville and the Caputo derivative.

Theorem 2.1.20. *Let $\alpha \geq 0$, n be the smallest integer greater than α (i.e. $n = \lceil \alpha \rceil$) and $f \in C^n[a,b]$, then*

$$^{GL}D_a^\alpha f(t) = \sum_{k=0}^{n-1} \frac{f^{(k)}(a)(t-a)^{k-\alpha}}{\Gamma(k+1-\alpha)} + \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-s)^{n-1-\alpha} f^{(n)}(s)ds. \qquad (2.16)$$

With the above theorem we can easily connect D_a^α, $^CD_a^\alpha$ and $^{GL}D_a^\alpha$ as follows

Corollary 2.1.21. *Let $\alpha \geq 0$, $n = \lceil \alpha \rceil$ and $f \in C^n[a,b]$. Then*

$$^{GL}D_a^\alpha f(t) = T_{n-1}[f;a](t) + {}^C D_a^\alpha f(t) = D_a^\alpha f(t),$$

where $T_{n-1}[f;a]$ denotes the Taylor polynomial of degree $n-1$ for the function f, centered at a.

Proof. The statment $^{GL}D_a^\alpha f(t) = T_{n-1}[f;a](t) + {}^C D_a^\alpha f(t)$ is a direct consequence of Theorem 2.1.20 and $T_{n-1}[f;a](t) + {}^C D_a^\alpha f(t) = D_a^\alpha f(t)$ has been proven in Theorem 2.1.15 (with the centered point a). $\qquad \square$

2.2 Fractional differential equations of Caputo-type

FDEs are generalizations of classical differential equations to an arbitrary (non-integer) order. The many important mathematical models are described by differential equations containing

fractional-order derivatives. Such models are interesting for engineers, biologists and physicists but also for pure mathematicians. Their evolutions behave in a much more complex way than in the classical integer-order case and the study of the corresponding theory is a hugely demanding task.

Before starting with the theory of FDEs, we shall consider a berief history of Volterra integral equation and the most simple integral equations of fractional order, namely the Abel integral equations of the first and the second kind.

2.2.1 Fractional integral equations

In general, an integral equation is a functional equation in which the unknown function appears under one or several integral signs like the Volterra integral equation. This subsection is devoted to an introduction to the theory of Volterra integral and its connections with the fractional integral.

Abel [1, 2] considered the *tautochrone problem*. That problem deals with the determination of the shape of the curve such that the time of descent of a frictionless point mass sliding down along the curve under the action of gravity is independent of the starting point. He showed that this problem can be described by a first-kind integral equation of the form

$$\int_0^t (t-s)^{-1/2} f(s) ds = k, \tag{2.17}$$

where f is the function to be determined and k is a constant. As Samko et al. pointed out in their book [155] it is important to note that Abel not only solved the integral equation (2.17) as the special case of the *tautochrone problem*, but instead gave the solution for the more general integral equation

$$g(t) = \int_0^t \frac{f(s)}{(t-s)^\alpha} ds, \quad t > 0, \quad 0 < \alpha < 1. \tag{2.18}$$

Such that Abel proved that, for $\alpha \in (0,1)$, the solution of (2.18) is given by the "inversion formula",

$$f(t) = c_\alpha \frac{d}{dt} \left\{ \int_0^t (t-s)^{\alpha-1} g(s) ds \right\}, \quad t > 0, \tag{2.19}$$

with $c_\alpha = \sin(\alpha\pi)/\pi \ (= 1/(\Gamma(\alpha)\Gamma(\alpha-1)))$.

Three years after Abel's death the problem of inverting (2.18) was also studied by Liouville [103]. In 1884 Sonine extended the inversion formula to cover first-kind integral equations characterized by convolution kernels, $a = a(t-s)$, given by

$$a(z) = z^{-\alpha} \sum_{j=0}^\infty \frac{c_j z^j}{\Gamma(1+j-\alpha)}, \quad c_0 = 1, \quad 0 < \alpha < 1.$$

Now let's go ahead to 1896, the year when Volterra published his general theory on the inversion of first-kind integral equations. Volterra [172] (Nota I) transforms the following equation (2.20),

$$\int_0^t K(t,s)f(s)ds = g(t), \quad t \in I = [0,T], \quad g(0) = 0, \tag{2.20}$$

by differentiation with respect to t, into an integral equation of the second kind whose kernel and forcing function are respectively, $\tilde{K}(t,s) := -(\partial K(t,s)/\partial t)/K(t,t)$ and $\tilde{g}(t) := g'(t)/K(t,t)$; if $K(t,t)$ does not vanish on I (closed and bounded interval with $0 < T$), and if the derivatives of K and g are continuous, then the (unique) solution of (2.20) is given by the "inversion formula"

$$f(t) = g(t) + \int_0^t \tilde{R}(t,s)g(s)ds, \quad t \in I.$$

Where, $\tilde{R}(t,s)$ denotes the so-called *resolvent kernel* of $\tilde{K}(t,s)$.

Even though Volterra's result was new, his way of attack was not entirely a novel one. In his thesis of 1894, Le Roux had already studied the problem of inverting the "definite integral" (2.20) (see Le Roux [99], p.243-246), using the same approach. But second-kind integral equations with variable limit of integration occur already in thr work of Liouville [1837](the name "Volterra integral equation" was coined by Lalesco [97]). In a second paper [172] (Nota II), Volterra extended his ideas to linear integral equations of first kind with weakly singular kernels: by using the approach employed by Abel to establish the inversion formula (2.19) he shows that

$$\int_0^t (t-s)^{-\alpha} K(t,s)f(s)ds = g(t), \quad t \in I, \quad 0 < \alpha < 1,$$

can be transformed into a first-kind equation with regular kernel, to which the theory of his first Nota applies.

Now, we can conclude that the former investigations on such equations (i.e. fractional integral equations) are due to Abel (1823-26), after whom they are named, for the first kind, and to Hille and Tamarkin (1930) for the second kind. The interested reader is referred to [31, 155, 74, 75, 76] for historical notes and detailed analysis with applications. Here we restrict ourselves to put some emphasis on the method of the Laplace transforms, that makes easier and more comprehensible the treatment of such fractional integral equations.

(I) Abel integral equation of the first kind:

Let us consider the Abel integral equation of the first kind

$$\frac{1}{\Gamma(\alpha)} \int_0^t \frac{u(s)}{(t-s)^{1-\alpha}} ds = f(t), \quad 0 < \alpha < 1, \tag{2.21}$$

where $f(t)$ is a given function. This may also be written as

$$I^\alpha u(t) = f(t),$$

and consequently solved in terms of a fractional derivative, according to

$$u(t) = D^\alpha f(t).$$

To this end we need to recall the definition fractional integral (2.4) and the property $D^\alpha I^\alpha = I$. Let us now solve (2.21) using the Laplace transform. Noting from (2.5) and (2.6), we obtain

$$\mathscr{L}\{I^\alpha u(t)\} = \mathscr{L}\{\phi_\alpha(t) * u(t)\} = \mathscr{L}\{f(t)\} \Rightarrow \widetilde{u}(s) = s^\alpha \widetilde{f}(s). \tag{2.22}$$

Now we can choose two different ways to get the inverse Laplace transform from (2.22), according to the standard rules. Writing (2.22) as

$$\widetilde{u}(s) = s \left[\frac{\widetilde{f}(s)}{s^{1-\alpha}} \right],$$

we obtain

$$u(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t \frac{f(s)}{(t-s)^\alpha} ds. \tag{2.23}$$

On the other hand, writing (2.22) as

$$\widetilde{u}(s) = \frac{1}{s^{1-\alpha}} [s\widetilde{f}(s) - f(0^+)] + \frac{f(0^+)}{s^{1-\alpha}},$$

we obtain

$$u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{f'(s)}{(t-s)^\alpha} ds + f(0^+) \frac{t^{-\alpha}}{\Gamma(1-\alpha)}. \tag{2.24}$$

Thus, the solutions (2.23) and (2.24) are expressed in terms of the fractional derivatives D^α and $^C D^\alpha$, respectively, according to (2.10) and (2.11) with $n = 1$.

(II) Abel integral equation of the second kind:

Let us now consider the Abel equation of the second kind

$$u(t) + \frac{\lambda}{\Gamma(\alpha)} \int_0^t \frac{u(s)}{(t-s)^{1-\alpha}} ds = f(t), \quad \alpha > 0, \quad \lambda \in \mathbb{C}. \tag{2.25}$$

In terms of the fractional integral operator such equation reads

$$(1 + \lambda I^\alpha) u(t) = f(t), \tag{2.26}$$

The solution to (2.26) is found to be

$$u(t) = (1 + \lambda I^\alpha)^{-1} f(t) = \left(1 + \sum_{m=1}^{\infty} (-\lambda)^m I^{\alpha m} \right) f(t). \tag{2.27}$$

Noting by (2.5) and (2.6) that

$$I^{\alpha m} f(t) = \phi_{\alpha m}(t) * f(t) = \frac{t_+^{\alpha m - 1}}{\Gamma(\alpha m)} * f(t),$$

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the formal solution reads

$$u(t) = f(t) + \left(\sum_{m=1}^{\infty} (-\lambda)^m \frac{t_+^{\alpha m - 1}}{\Gamma(\alpha m)} \right) * f(t). \tag{2.28}$$

From Definition 1.2.10, we can show that

$$e_\alpha(t; \lambda) := E_\alpha(-\lambda t^\alpha) = \sum_{m=0}^{\infty} \frac{(-\lambda t^\alpha)^m}{\Gamma(\alpha m + 1)}, \ t > 0, \ \alpha > 0, \ \lambda \in \mathbb{C},$$

where E_α denotes the Mittag-Leffler function of order α, we note that

$$\sum_{m=1}^{\infty} (-\lambda)^m \frac{t_+^{\alpha m - 1}}{\Gamma(\alpha m)} = \frac{d}{dt} E_\alpha(-\lambda t^\alpha) = e_\alpha'(t; \lambda), \ t > 0.$$

Thus, the solution to the integral equation of the second kind can be formally written as

$$u(t) = f(t) + e_\alpha'(t; \lambda) * f(t). \tag{2.29}$$

The same solution can be reached by using Laplace transform. Start by taking the laplace transform of (2.25)

$$\left[1 + \frac{\lambda}{s^\alpha} \right] \widetilde{u}(s) = \widetilde{f}(s) \Rightarrow \widetilde{u}(s) = \frac{s^\alpha}{s^\alpha + \lambda} \widetilde{f}(s). \tag{2.30}$$

As for the Abel equation of the first kind, we can choose two different ways to get the inverse Laplace transforms from (2.30), according to the standard rules. Writing (2.30) as

$$\widetilde{u}(s) = s \left[\frac{s^{\alpha - 1}}{s^\alpha + \lambda} \widetilde{f}(s) \right],$$

we obtain

$$u(t) = \frac{d}{dt} \int_0^t f(t - s) e_\alpha(s; \lambda) ds. \tag{2.31}$$

If we write (2.30) as

$$\widetilde{u}(s) = \frac{s^{\alpha - 1}}{s^\alpha + \lambda} [s \widetilde{f}(s) - f(0^+)] + f(0^+) \frac{s^{\alpha - 1}}{s^\alpha + \lambda},$$

we obtain

$$u(t) = \int_0^t f'(t - s) e_\alpha(s; \lambda) ds + f(0^+) e_\alpha(s; \lambda). \tag{2.32}$$

We also note that, $e_\alpha(s; \lambda)$ being a function differentiable with respect to t with $e_\alpha(0^+; \lambda) = E_\alpha(0^+) = 1$, there exists another possibility to re-write (2.30), namely

$$\widetilde{u}(s) = \left[s \frac{s^{\alpha - 1}}{s^\alpha + \lambda} - 1 \right] \widetilde{f}(s) + \widetilde{f}(s).$$

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Then we obtain

$$u(t) = \int_0^t f(t-s)e'_\alpha(s;\lambda)ds + f(t), \qquad (2.33)$$

in agreement with (2.29).

2.2.2 Existance and uniqueness theorems

At the beginning of this part we give a brief overview of the results of existence and uniqueness theorems for ordinary differential equations involving Caputo fractional derivative on a finite interval of the real axis. Then, we will discuss some properties for the solution of these equation but we restrict ourselves to initial value problems (Cauchy problems) and furthermore we assume without loss of generality that the Caputo fractional derivative is developed at the point 0.

To illustrate the main advantage of considering the Caputo fractional derivative, Let the following initial value problems

$$\begin{aligned} D^\alpha y(t) - \lambda y(t) &= 0, \quad t > 0, \ n-1 < \alpha < n \in \mathbb{N}, \ \lambda > 0 \\ D^{\alpha-k-1} y(t)|_{t=0} &= b_k, \quad k = 0,1,...,n-1 \end{aligned} \qquad (2.34)$$

and

$$\begin{aligned} {}^C D^\alpha y(t) - \lambda y(t) &= 0, \quad t > 0, \ n-1 < \alpha < n \in \mathbb{N}, \ \lambda > 0 \\ y^{(k)}(0) &= b_k, \quad k = 0,1,...,n-1. \end{aligned} \qquad (2.35)$$

In (2.34) the Riemann-Liouville fractional differentiation operator is applicable. In this case, also in the initial conditions fractional derivatives are required. Such initial value problems can successfuly be solved theoretically, but their solutions are practically useless, because there is no clear physical interpretation of this type of initial conditions (see [141], p.78). On the contrary, in (2.35) where the Caputo fractional differentiation operator is applicable, standard initial conditions in terms of derivatives of integer order are involved. These initial conditions have clear physical interpretation as an initial position $y(a)$ at the point a (where y is the unknown function), the initial velocity $y'(a)$, initial acceleration $y''(a)$ and so on. On the other hand, the Caputo fractional derivative is more restrictive, as it can be seen from (2.10) and (2.11), since it requires the existence of the $n-$derivative of the function. Fortunately, most functions that appear in applications fulfill this requirement. Later, whenever the Caputo operator is used, it is assumed that this condition is satisfied.

Now, we go back to the goals in this part where FDEs with Caputo fractional derivative are studied extensively. Gorenflo and Mainardi [69] applied the Laplace transform to solve the FDE

$$(\ {}^C D_{0+}^\alpha y)(x) - \lambda y(x) = f(x), \ x > 0; \ \alpha > 0; \ \lambda > 0, \qquad (2.36)$$

with the Caputo fractional derivative of order $\alpha > 0$ and with the initial conditions

$$y^{(k)}(0) = b_k \ , k = 0,1,...,n-1; \ n-1 < \alpha \leq n; \ n \in \mathbb{N}. \qquad (2.37)$$

They discussed the key role of the Mittag-Leffler function for the cases $1 < \alpha < 2$ and $2 < \alpha < 3$. In this regard, see also the papers by Gorenflo and Mainardi [70], Gorenflo and Rutman [71], and Gorenflo et al. [72]. Luchko and Gorenflo [118] used the operational method to prove that the Cauchy problem (2.36)-(2.37) has the unique solution

$$y(x) = \sum_{k=0}^{n-1} b_k x^k E_{\alpha, k+1}(\lambda x^\alpha) + \int_0^x (x-t)^{\alpha-1} E_{\alpha, \alpha}(\lambda(x-t)^\alpha) f(t) dt,$$

in terms of the Mittag-Lefler functions (1.13) in a special space of functions on the half-axis $\mathbb{R}_+$. They also obtained the explicit solution to the Cauchy problem for the more general FDE.

Diethelm and Ford [53] investigated the Cauchy problem for the nonlinear differential equation of order $\alpha > 0$

$$({}^C D_{0+}^\alpha y)(x) = f(x, y(x)), \quad 0 \le x \le b < \infty, \tag{2.38}$$

with initial conditions (2.37). They proved the uniqueness and existence of a local continuous solution $y(x) \in C[0, h]$ to this problem for continuous and Lipschitzian f; in this regard, see also Diethelm ([54], Theorems 5.4-5.5). The dependence of this solution $y(x)$ on the order α, on the initial data (2.37), and on the function f was investigated. Applications were given to present numerical schemes for the solution $y(x)$ to the simplest linear problem with $0 < \alpha < 1$:

$$({}^C D_{0+}^\alpha y)(x) = \lambda y(x) + f(x), \quad (0 \le x \le b; \ \lambda < 0), \quad y(0) = b \in \mathbb{R}. \tag{2.39}$$

Kilbas and Marzan ([90] and [91]) investigated the Cauchy problem of the form (2.38)-(2.37) with the Caputo derivative of complex order $\alpha \in \mathbb{C}$ $(Re(\alpha) > 0)$:

$$({}^C D_{0+}^\alpha y)(x) = f(x, y(x)), \quad 0 \le x \le b, \tag{2.40}$$

$$y^{(k)}(0) = b_k \in \mathbb{C} \quad k = 0, 1, ..., n-1, \tag{2.41}$$

where $n = [Re(\alpha)] + 1$ for $\alpha \notin \mathbb{N}$ and $n = \alpha$ for $\alpha \in \mathbb{N}$, on a finite interval $[a, b]$ of $\mathbb{R}$. They proved the equivalence of (2.39)-(2.38) and the Volterra integral equation of second kind of the following form

$$y(x) = \sum_{k=0}^{n-1} \frac{b_k}{\Gamma(k+1)} (x-a)^k + \frac{1}{\Gamma(\alpha)} \int_a^x \frac{f(t, y(t)) \, dt}{(x-t)^{1-\alpha}}, \quad x > a$$

in the space $C^{n-1}[a, b]$ and applied this result to establish conditions for a unique solution $y(x) \in C^{n-1}[a, b]$ to the Cauchy problem (2.40)-(2.41).

From the above results, we give the formal definition of a FDE involving Caputo fractional derivative and discuss existance, uniqueness properties.

Definition 2.2.1. Let $\alpha > 0$, $\alpha \notin \mathbb{N}$, $n = \lceil \alpha \rceil$ and $f : A \subseteq \mathbb{R}^2 \to \mathbb{R}$. Then

$${}^C D^\alpha y(t) = f(t, y(t)) \tag{2.42}$$

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is called fractional differential equation of Caputo type. As initial conditions for this type of FDE be

$$D^k y(0) = y^{(k)}(0) = b_k, \quad (k = 0, 1, ..., n - 1). \tag{2.43}$$

We now have the following theorem (see e.g. [39])

Theorem 2.2.2. *Let $\alpha > 0$, $\alpha \notin \mathbb{N}$ and $n = \lceil \alpha \rceil$. Moreover, let $b_0, b_1, ..., b_{n-1} \in \mathbb{R}$, $K > 0$ and $h^* > 0$. Define*

$$G = [0, h^*] \times [b_0 - K, b_0 + K],$$

and let the function $f : G \to \mathbb{R}$ be continuous. Then, there exists some $h > 0$ and a function $y \in C[0, h]$ solving the fractional differential equation of Caputo type (2.42) combined with initial conditions (2.43). For the case $\alpha \in (0, 1)$ the parameter h is given by

$$h := \min\{h^*, (K\Gamma(\alpha + 1)/M)^{1/\alpha}\}, \quad with \quad M := \sup_{(t,z)\in G} |f(t, z)|.$$

If furthermore f fulfils a Lipschitz condition with respect to the second variable, i.e.

$$|f(t, y_1) - f(t, y_2)| \leq L|y_1 - y_2|$$

with some constant $L > 0$ independent of t, y_1, and y_2, the function $y \in C[0, h]$ is unique.

To prove the Theorem 2.2.2, we will use the following lemma to show that this type of FDE can formulated as an integral equation, namely Volterra integral equation:

Lemma 2.2.3. *Assume the hypotheses of Theorem 2.2.2. The function $y \in C[0, h]$ is a solution of the fractional differential equation of Caputo type (2.42), combined with the initial conditions (2.43) if and only if it is a solution of the nonlinear Volterra integral equation of the second kind*

$$y(t) = \sum_{k=0}^{n-1} \frac{t^k}{k!} b_k + \frac{1}{\Gamma(\alpha)} \int_0^t (t - s)^{\alpha-1} f(s, y(s)) ds. \tag{2.44}$$

Before we are going to prove this lemma, there is comment which we can understand by using formula (2.44) the importance of non-locality for fractional operator.

Remark 2.2.4. Let us consider formula (2.44) for some $\alpha \in (0, 1]$ (i.e. $n = 1$) and for two different values of t, say t_1 and t_2 with $t_1 < t_2$, then we can write

$$
\begin{aligned}
y(t_2) - y(t_1) &= \frac{1}{\Gamma(\alpha)} \int_0^{t_1} [(t_2 - s)^{\alpha-1} - (t_1 - s)^{\alpha-1}] f(s, y(s)) ds \\
&\quad + \frac{1}{\Gamma(\alpha)} \int_{t_1}^{t_2} (t_2 - s)^{\alpha-1} f(s, y(s)) ds.
\end{aligned} \tag{2.45}
$$

(I) In the classical case $\alpha = 1$, the term in brackets on the right-hand side of (2.45) is zero, hence the entire first integral vanishes and we have

$$y(t_2) - y(t_1) = \int_{t_1}^{t_2} f(s, y(s))ds,$$

this implies that, if we already know the solution $y(t_1)$ of our given problem (2.42) with (2.43) at the point $t_1 > 0$, then we may compute the solution at the point $t_2 > t_1$ exclusively on the basis of $y(t_1)$ and the function f. We do not need to use any information on $y(t)$ for $t \in [0, t_1)$. This observation is the basis of almost all classical methods for the numerical solution of first-order differential equations, and it is also of fundamental significance in the mathematical modelling of many systems in biology, physics, engineering, and other sciences because it states that it is sufficient to observe the state of a first-order system at an arbitrary point in time to compute its behaviour in the future.

(II) In the fractional case $0 < \alpha < 1$, this situation is fundamentally different. Here the first integral on the right-hand side of (2.45) does not vanish in general. Hence, whenever we want to compute the solution $y(t_2)$ at some point t_2 it is necessary to take into account the entire history of y from the starting point 0 up to the point of interest t_2. This reflects the non-locality of the Caputo fractional differential operator.

It thus follows that integer-order equations are appropriate tools for the modelling of systems without memory whereas fractional-order equations are the method of choice for the description of systems with memory.

Proof. (of Lemma 2.2.3) We want to prove that every continuous solution of the Volterra equation (2.44) is also solution of the initial value problem (2.42), (2.43). By using Corollary 2.1.16 we can rewrite the FDE (2.42) to

$$f(t, y(t)) = {}^{C}D^{\alpha}y(t) = D^{\alpha}(y - T_{n-1}[y; 0])(t) = D^{n}I^{n-\alpha}(y - T_{n-1}[y; 0])(t).$$

Since we are dealing with continuous functions, we can integrate n-times on both sides and get

$$I^{n}f(t, y(t)) = I^{n-\alpha}(y - T_{n-1}[y; 0])(t) + q(t),$$

where $q(t)$ is a polynomial of degree not exceeding $n - 1$. Since $f(t, y(t))$ is continuous, the function $I^{n}f(t, y(t))$ on the left-hand side of this equation has an n-fold zero at the origin. By definition of the Taylor polynomial, the difference $y - T_{n-1}[y; 0]$ has the same property by construction, and therefore the function $I^{n-\alpha}(y - T_{n-1}[y; 0])(t)$ on the right-hand side of our equation must have such an mth order zero too. Hence $q(t) = 0$ and consequently

$$I^{n}f(t, y(t)) = I^{n-\alpha}(y - T_{n-1}[y; 0])(t).$$

Applying the Riemann-Liouville operator $D^{n-\alpha}$ on both sides of the equation yields

$$I^{\alpha}f(t, y(t)) = y(t) - T_{n-1}[y; 0](t),$$

where the Taylor polynomial (with initial conditions (2.43))

$$T_{n-1}[y; 0] = \sum_{k=0}^{n-1} \frac{t^k}{k!} b_k,$$

this is just the required Volterra integral equation. $\qquad\square$

With this the result we can now prove analogues to the Theorems 2.2.2, where we see that our initial value problem (2.42) and (2.43) is equivalent to the Volterra integral equation.

Lemma 2.2.5. *Under the assumptions of Theorem 2.2.2, the Volterra equation (2.44) possesses a uniquely determined solution $y \in C[0, h]$.*

Proof. We divide the proof in two parts. First we consider the case $\alpha > 1$ and secondly the case $\alpha \in (0, 1)$. The reasoning behind this lies in the fact that the Volterra integral equation (2.44) possesses a singular kernel $(t - s)^{\alpha-1}$ in the case $\alpha \in (0, 1)$, while the kernel is continuous in the other case.

Case $\alpha > 1$: The equation (2.44) possesses a continuous kernel and a continuous given function outside the integral. Thus the existence of the solution follows using standard methods from the theory of Volterra equations [131]. Similarly by using the Lipschitz condition the uniqueness can be proven directly with standard methods from the theory of Volterra equations [131].

Case $\alpha \in (0, 1)$: In this situation, the Volterra equation (2.44) reduces to

$$y(t) = b_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t - s)^{\alpha-1} f(s, y(s)) ds. \tag{2.46}$$

Existance of solution :
For the proof of the existence of a solution we introduce the set $U := \{y \in C[0, h] : \|y - b_0\|_\infty \leq K\}$. It is evident that U is a closed and convex subset of the Banach space of all continuous functions on $[0, h]$, equipped with the Chebyshev norm. Hence, U is a Banach space too. Since the constant function $y \equiv b_0$ is in U, we also see that U is not empty. On this set U we define the operator A by

$$(Ay)(t) := b_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t - s)^{\alpha-1} f(s, y(s)) ds. \tag{2.47}$$

Using this operator, the equation under consideration can be rewritten as $y = Ay$, and thus, in order to prove our desired existence result, we have to show that A has a fixed point. Let us therefore investigate the properties of the operator A.

First we want to show that $Ay \in U$ for $y \in U$. To this end we begin by noting that, for

$0 \leq t_1 \leq t_2 \leq h$,

$$
\begin{aligned}
|(Ay)(t_1) - (Ay)(t_2)| &= \frac{1}{\Gamma(\alpha)} \left| \int_0^{t_1} (t_1 - s)^{\alpha-1} f(s, y(s)) ds - \int_0^{t_2} (t_2 - s)^{\alpha-1} f(s, y(s)) ds \right| \\
&= \frac{1}{\Gamma(\alpha)} \left| \int_0^{t_1} [(t_1 - s)^{\alpha-1} - (t_2 - s)^{\alpha-1}] f(s, y(s)) ds \right. \\
&\quad + \left. \int_{t_1}^{t_2} (t_2 - s)^{\alpha-1} f(s, y(s)) ds \right| \\
&\leq \frac{\|f\|_\infty}{\Gamma(\alpha)} \left| \int_0^{t_1} [(t_1 - s)^{\alpha-1} - (t_2 - s)^{\alpha-1}] ds + \int_{t_1}^{t_2} (t_2 - s)^{\alpha-1} ds \right|
\end{aligned}
$$

The second integral in the right-hand side of above equation has the value $(t_2 - t_1)^\alpha/\alpha$. but the first integral, for $\alpha < 1$, we have $\alpha - 1 < 0$, and hence $(t_1 - s)^{\alpha-1} \geq (t_2 - s)^{\alpha-1}$. Thus,

$$
\int_0^{t_1} |(t_1 - s)^{\alpha-1} - (t_2 - s)^{\alpha-1}| ds = \frac{1}{\alpha}(t_1^\alpha - t_2^\alpha + (t_2 - t_1)^\alpha) \leq \frac{1}{\alpha}(t_2 - t_1)^\alpha. \tag{2.48}
$$

And we can write

$$
|(Ay)(t_1) - (Ay)(t_2)| \leq \frac{\|f\|_\infty}{\Gamma(\alpha+1)}(2(t_2 - t_1)^\alpha + t_1^\alpha - t_2^\alpha). \tag{2.49}
$$

The expression on the right-hand side of (2.49) converges to 0 as $t_2 \to t_1$ which proves that Ay is a continuous function. Moreover, for $y \in U$ and $t \in [0, h]$, we find

$$
\begin{aligned}
\left| (Ay)(t) - y_0^{(0)} \right| &= \frac{1}{\Gamma(\alpha)} \left| \int_0^t (t - s)^{\alpha-1} f(s, y(s)) ds \right| \leq \frac{1}{\Gamma(\alpha+1)} \|f\|_\infty t^\alpha \\
&\leq \frac{1}{\Gamma(\alpha+1)} \|f\|_\infty h^\alpha \leq \frac{1}{\Gamma(\alpha+1)} \|f\|_\infty \frac{K\Gamma(\alpha+1)}{\|f\|_\infty} = K.
\end{aligned}
$$

Thus, we have shown that $Ay \in U$ if $y \in U$, i.e. A maps the set U to itself.

Since we want to apply Schauder's Fixed Point Theorem (Theorem 1.1.13), all that remains now is to show that $A(U) := \{Au : u \in U\}$ is a relatively compact set. This can be done by means of the Arzelà-Ascoli Theorem (Theorem 1.1.15). For $z \in A(U)$ we find that, for all $t \in [0, h]$,

$$
\begin{aligned}
|z(t)| &= |(Ay)(t)| \leq |b_0| + \frac{1}{\Gamma(\alpha)} \int_0^t (t - s)^{\alpha-1} |f(s, y(s))| ds \\
&\leq |b_0| + \frac{1}{\Gamma(\alpha+1)} \|f\|_\infty h^\alpha,
\end{aligned}
$$

which is the required boundedness property. Moreover, for $0 \leq t_1 \leq t_2 \leq h$ (the equicontinuity property), from equations (2.49) and (2.48) we have

$$
\begin{aligned}
|(Ay)(t_1) - (Ay)(t_2)| &\leq \frac{\|f\|_\infty}{\Gamma(\alpha+1)}(2(t_2 - t_1)^\alpha + t_1^\alpha - t_2^\alpha) \\
&\leq 2\frac{\|f\|_\infty}{\Gamma(\alpha+1)}(t_2 - t_1)^\alpha.
\end{aligned}
$$

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Thus, if $|t_2 - t_1| < \delta$, then

$$|(Ay)(t_1) - (Ay)(t_2)| \leq 2\frac{\|f\|_\infty}{\Gamma(\alpha + 1)}\delta^\alpha.$$

Noting that the expression on the right-hand side is independent of y, we see that the set $A(U)$ is equicontinuous. Then, the Arzelà-Ascoli Theorem yields that $A(U)$ is relatively compact, and hence Schauder's Fixed Point Theorem asserts that A has a fixed point. By construction, a fixed point of A is a solution of our initial value problem.

Uniqueness of solution :
For the uniqueness of the solution we use the same operator A (defined in (2.47)) and recall that it maps the nonempty, convex and closed set $U = \{y \in C[0, h] : \|y - b_0\|_\infty \leq K\}$ to itself. We now have to prove that A has a unique fixed point. In order to do this, we shall first prove that, for every $j \in \mathbb{N}_0$, every $t \in [0, h]$ and all $y, \bar{y} \in U$, we have

$$\|A^j y - A^j \bar{y}\|_{L_\infty[0,t]} \leq \frac{(Lt^\alpha)^j}{\Gamma(1 + \alpha j)}\|y - \bar{y}\|_{L_\infty[0,t]}. \tag{2.50}$$

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

$$\begin{aligned}
\|A^j y - A^j \bar{y}\|_{L_\infty[0,t]} &= \|A(A^{j-1}y) - A(A^{j-1}\bar{y})\|_{L_\infty[0,t]} \\
&= \frac{1}{\Gamma(\alpha)}\sup_{0 \leq w \leq t}\left|\int_0^w (w - s)^{\alpha-1}[f(s, A^{j-1}y(s)) - f(s, A^{j-1}\bar{y}(s))]ds\right|.
\end{aligned}$$

In the next steps, we use the Lipschitz assumption on f and the induction hypothesis. This allows us to estimate the quantities under consideration in the following way:

$$\begin{aligned}
\|A^j y - A^j \bar{y}\|_{L_\infty[0,t]} &\leq \frac{L}{\Gamma(\alpha)}\sup_{0 \leq w \leq t}\int_0^w (w - s)^{\alpha-1}|A^{j-1}y(s) - A^{j-1}\bar{y}(s)|ds \\
&\leq \frac{L}{\Gamma(\alpha)}\int_0^t (t - s)^{\alpha-1}\sup_{0 \leq w \leq s}|A^{j-1}y(w) - A^{j-1}\bar{y}(w)|ds \\
&\leq \frac{L^j}{\Gamma(\alpha)\Gamma(1 + \alpha(j-1))}\int_0^t (t - s)^{\alpha-1}s^{\alpha(j-1)}\sup_{0 \leq w \leq s}|y(w) - \bar{y}(w)|ds \\
&\leq \frac{L^j}{\Gamma(\alpha)\Gamma(1 + \alpha(j-1))}\sup_{0 \leq w \leq t}|y(w) - \bar{y}(w)|\int_0^t (t - s)^{\alpha-1}s^{\alpha(j-1)}ds \\
&= \frac{L^j}{\Gamma(\alpha)\Gamma(1 + \alpha(j-1))}\|y - \bar{y}(w)\|_{L_\infty[0,t]}\frac{\Gamma(\alpha)\Gamma(1 + \alpha(j-1))}{\Gamma(1 + \alpha j)}t^{\alpha j}.
\end{aligned}$$

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which is our desired result (2.50). As a consequence, we find, taking Chebyshev norms on our fundamental interval $[0, h]$,

$$\|A^j y - A^j \bar{y}\|_\infty \leq \frac{(Lh^\alpha)^j}{\Gamma(1+\alpha j)}\|y - \bar{y}\|_\infty.$$

We have now shown that the operator A fulfils the assumptions of Theorem 1.1.11 with $\alpha_j = (Lh^\alpha)^j/\Gamma(1+\alpha j)$. In order to apply that theorem, we only need to verify that the series $\sum_{j=0}^\infty \alpha_j$ converges. To this end we notice that $\sum_{j=0}^\infty \alpha_j$ with α_j as above is simply the power series representation of the Mittag-Leffler function $E_\alpha(Lh^\alpha)$, and hence the required convergence of the series follows immediately from Theorem 1.2.11. Therefore, we may apply Weissinger's Fixed Point Theorem and deduce the uniqueness of the solution of our differential equation. $\qquad \square$

2.2.3 Properties of the solution

An important and frequently used result in the theory of equations was the equivalence between the initial value problem (2.42)-(2.43) and corresponding Volterra integral equation. In fact, equation (2.44) is a special case of the more general weakly singular Volterra equation which is given by the following formal definition.

Definition 2.2.6. An equation of the form

$$y(t) = g(t) + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} K(t, s, y(s))ds, \quad t \in [0, T] \tag{2.51}$$

with $\alpha > 0$ and some $T > 0$ is called Volterra integral equation with weak singularity in the kernel.

In various places in the literature one can find the statement that ordinary fractional differential equations with Caputo-type differential operators with smooth right-hand sides $f(t, y(t))$ cannot have smooth solutions. More precisely, Miller and Feldstein in [132] also Lubich in [115] showed that the solutions of IVP (2.42)-(2.43) will not be smooth (as functions of the independent variable t only) in general, even if f is smooth and a fundamental remark in ([115], p.89) states that it is not possible for f and the solution y to be smooth at 0 simultaneously.

We can conclude that, the problems considered so far have all been regular in the sense that the function f on the right-hand side of the differential equation (2.42) has been at least continuous (and, in most cases, even differentiable a certain number of times). In some applications however one encounters equations where this is not the case. Therefore we will now show the significance of the continuity assumption for the right-hand side f. To this end, we look at the following examples.

Example 2.2.7. For $\alpha \in (1, 2)$ consider the initial value problem

$$^C D^\alpha y(t) = \frac{1}{y(t) - 1}, \quad y(0) = 1, \ y'(0) = 0. \tag{2.52}$$

If we ignore the discontinuity of $f(t,y) = (y-1)^{-1}$ at the initial point $(t_0, y_0) = (0, 1)$ and apply the standard theory for continuous f, then we arrive at the integral equation

$$y(t) = 1 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} \frac{1}{y(s)-1} ds. \qquad (2.53)$$

Equation (2.53) is solved by the functions

$$y(t) = 1 \pm \frac{\sqrt{\Gamma(1-\alpha/2)}}{\sqrt{\Gamma(1+\alpha/2)}}, \qquad (2.54)$$

which is readily verified by substitution.

Example 2.2.8. Consider the following problem such that $n = \lceil \alpha \rceil$

$$^C D^\alpha y(t) = 1 - y(t), \quad y_0^{(0)} = 1, \ y_0^{(k)} = 0 \ (k = 1, 2, ..., n-1). \qquad (2.55)$$

The solution of this problem is $y(t) \equiv 1$.

Two points are important to note from these examples:

(a) We observe in the context of Example 2.2.7 that the integral equation formulation has more than one continuous solution. However, both these solutions have unbounded first derivatives at $t = 0$, and therefore these solutions do not satisfy the second initial condition of (2.52) (i.e. in the presence of singularities we may lose the equivalence).

(b) In Example 2.2.8, both f and y are entire functions. Consequently, we know now why the version of Theorem 2, in [115], given by Lubich goes wrong.

We now try to give a precise account of the situations in which simultaneous analyticity of f and the solution y can occur, and for more details refer to [50].

Theorem 2.2.9. *Consider the initial value problem (2.42)-(2.43) with $\alpha > 0$, $\alpha \notin \mathbb{N}$ and $n = \lceil \alpha \rceil$. Let the function g be defined with the help of the given initial values as*

$$g(t) := \sum_{k=0}^{n-1} \frac{y_0^{(k)}}{k!} t^k,$$

(i.e. g is the Taylor polynomial of degree $n-1$ of y at the point 0). Assume that f is analytic on $[0, T] \times G$, where $G \subset \mathbb{R}$ contains the range of g on $[0, T]$. Then, y is analytic if and only if $f(t, g(t)) = 0$ for all $t \in [0, T]$.

Theorem 2.2.9 shows that the occurence of an analytic solution to an equation of the form (2.42) with analytic right-hand side is a rare event. Nevertheless it can be used as guideline to construct problems with smooth solutions, for example if one needs test cases for numerical algorithms (as we will see in Chapter 3).

Proof. We first note that the analyticity of f implies the existence of a unique solution on some interval $[0, T]$, with $T > 0$.

The direction ($\Leftarrow$) can be seen in the following way. In view of (2.44), the condition $f(t, g(t)) \equiv 0$ implies that a solution of the initial value problem is $y = g$. Since g (and hence also y) is a polynomial, we have an analytic solution.

For ($\Rightarrow$) we assume y to be analytic. Then, since f is analytic at $(0, g(0))$, the function $z : [0, T] \to \mathbb{R}$ with $z(t) := f(t, y(t))$ is analytic at 0 because of $y(0) = g(0)$. Hence we can represent it in the form

$$z(t) = \sum_{k=0}^{\infty} z_k t^k,$$

with certain coefficients z_k. It follows from (2.44) that

$$\sum_{k=n}^{\infty} \frac{y_0^{(k)}}{k!} t^k = y(t) - \sum_{k=0}^{n-1} \frac{y_0^{(k)}}{k!} t^k = I^\alpha z(t) = \sum_{k=0}^{\infty} \frac{\Gamma(k+1)}{\Gamma(k+1+\alpha)} z_k t^{k+\alpha}. \qquad (2.56)$$

The left-hand side of (2.56) clearly is an analytic function at the point 0, so its right-hand side must be analytic there too. Since we assumed $\alpha \notin \mathbb{N}$, this is true if and only if $z_k = 0$ for all k, which is equivalent to saying that $0 = z(t) = f(t, y(t))$ for all t. Thus the integral equation form (2.44) of our initial value problem reduces to

$$y(t) = g(t) + I^\alpha z(t) = g(t),$$

and hence we have, for all t,

$$0 = f(t, y(t)) = f(t, g(t)).$$

$\square$

An inspection of the proof of Theorem 2.2.9 immediately reveals another important property:

(a) Assume the hypotheses of Theorem 2.2.9. If the given initial value problem has an analytic solution y then $y = g$, i.e. y is the polynomial from the kernel of the Caputo differential operator that fits the initial conditions.

(b) Consider the IVP (2.42)-(2.43) with $\alpha > 0$ and $\alpha \notin \mathbb{N}$. If the solution y of this problem is analytic but not a polynomial then the function f is not analytic.

A simple example clarifies these results:

Example 2.2.10. Consider the integral equation

$$y(t) = t + 1 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1}(y - s - 1)ds,$$

with non-integer α and $1 < \alpha < 2$. This equation corresponds to the initial value problem

$$^C D^\alpha y(t) = y(t) - t - 1, \quad y(0) = 1, \ y'(0) = 1,$$

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and is solved by

$$y(t) = t + 1,$$

which is an analytic function itself.

If we do not want to require the given function f to be analytic then we can still prove some useful results about the differentiability properties of the solution of the IVP (2.42)-(2.43) on the interval where the solution exists. For convenience we note that equation (2.44) reads

$$y(t) = p(t) + I^\alpha[f(., y(.))](t) \tag{2.57}$$

with p being some polynomial whose precise form is not of interest at the moment.

Theorem 2.2.11. *Consider the initial value problem (2.42)-(2.43) with $\alpha > 0$, $n = \lceil \alpha \rceil$ and f being continuous and satisfying a Lipschitz condition with respect to its second variable. Then, the solution y satisfies $y \in C^{n-1}[0, T]$.*

Proof. Let $k \in \{0, 1, 2..., n-1\}$ (this implies $k < \alpha$) and differentiate equation (2.57) k times:

$$
\begin{aligned}
D^k y(t) &= D^k p(t) + D^k I^\alpha[f(., y(.))](t) \\
&= D^k p(t) + D^k I^k I^{\alpha-k}[f(., y(.))](t) \\
&= D^k p(t) + I^{\alpha-k}[f(., y(.))](t)
\end{aligned}
$$

in view of some properties of fractional integration and the classical fundamental theorem of calculus. Now recall that y is continuous; thus the argument of the integral operator $I^{\alpha-k}$ is a continuous function. Hence, in view of the polynomial structure of p and the well known mapping properties of $I^{\alpha-k}$, the function on the right-hand side of the equation is continuous, and so the function on the left, viz. $D^k y$, must be continuous too. $\square$

Theorem 2.2.12. *Assume the hypotheses of Theorem 2.2.11. Moreover let $\alpha > 1$, $\alpha \notin \mathbb{N}$ and $f \in C^1(G)$ with $G = [y_0^{(0)} - K, y_0^{(0)} + K] \times \mathbb{R}$; $K > 0$. Then $y \in C^n(0, T]$. Furthermore, $y \in C^n[0, T]$ if and only if $f(0, y_0^{(0)}) = 0$.*

Remark 2.2.13. Since the function f and the initial value $y_0^{(0)}$ are given, it is easy to check whether the condition $f(0, y_0^{(0)}) = 0$ is fulfilled or not.

Remark 2.2.14. In the case of integer-order differential equations we well known the following theorem (also see Theorem 1.1.20)

Theorem 2.2.15. Let $k \in \mathbb{N}$ and $f \in C^{k-1}(G)$, where $G = [y_0 - K, y_0 + K] \times \mathbb{R}$. Then, the solution y of the initial value problem (1.6) is k-times continuously differentiable.

Thus, smoothness of the given function f implies smoothness of the solution y on the closed interval $[0, T]$; however in the fractional setting this holds only under certain additional conditions. In order to ensure this remark, we give the following example

Example 2.2.16. The non-differentiable function y given by $y(t) = t^{1/2}$ is the unique solution of the initial value problem $^C D^{1/2} y(t) = \Gamma(3/2)$, $y(0) = 0$, whose given function f (the right-hand side of the differential equation) is analytic.

Proof. (of Theorem 2.2.12) We introduce the abbreviation $z(t) := f(t, y(t))$ and differentiate equation (2.57) $k = n - 1$ we have:

$$
\begin{aligned}
D^{n-1} y(t) &= D^{n-1} p(t) + I^{\alpha-n+1} z(t) \\
&= D^{n-1} p(t) + \frac{1}{\Gamma(\alpha - n + 1)} \int_0^t (s - t)^{\alpha-n} z(s) ds.
\end{aligned}
$$

We differentiate once again, recall that p is a polynomial of degree $n - 1$ and find

$$
\begin{aligned}
D^n y(t) &= D^n p(t) + \frac{1}{\Gamma(\alpha - n + 1)} \frac{d}{dt} \int_0^t (t - s)^{\alpha-n} z(s) ds \\
&= \frac{1}{\Gamma(\alpha - n + 1)} \frac{d}{dt} \int_0^t (u)^{\alpha-n} z(t - u) du \\
&= \frac{1}{\Gamma(\alpha - n + 1)} \left(t^{\alpha-n} z(0) + \int_0^t (u)^{\alpha-n} z'(t - u) du \right).
\end{aligned}
$$

Thus, we have

$$
D^n y(t) = \frac{1}{\Gamma(\alpha - n + 1)} t^{\alpha-n} f(0, y_0^{(0)}) + I^{\alpha-n+1} z'(t). \tag{2.58}
$$

Since $\alpha > 1$ we deduce that $n \geq 2$, and thus Theorem 2.2.11 asserts that $y \in C^1[0, T]$. An explicit calculation gives that

$$
z'(t) = \frac{\partial}{\partial t} f + \frac{\partial}{\partial y} f y'(t).
$$

Consequently, by our differentiability assumption on f, the function z' is continuous, and so $I^{\alpha-n+1} z'(t) \in C[0, T]$ too (see e.g. [39]). The fact that $n > \alpha$ then finally yields that the right-hand side of (2.58), and therefore also the left-hand side of this equation, i.e. the function $D^n y$, is always continuous on the half-open interval $(0, T]$ whereas it is continuous on the closed interval $[0, T]$ if and only if $f(0, y_0^{(0)}) = 0$. $\qquad\square$

It is possible to generalize this idea and to keep Remarks 2.2.13 and 2.2.14 valid:

Theorem 2.2.17. *Assume the hypotheses of Theorem 2.2.11. Moreover let $k \in \mathbb{N}$, $\alpha > k$, $\alpha \notin \mathbb{N}$ and $f \in C^k(G)$. Let $z(t) := f(t, y(t))$. Then $y \in C^{n+k-1}(0, T]$. Furthermore, $y \in C^{n+k-1}[0, T]$ if and only if z has a k-fold zero at the origin.*

Proof. The proof is based on a repeated the arguments used in the proof of Theorem 2.2.12 (i.e. by repeating the differentiation of equation (2.58)). $\qquad\square$

A common feature of the results above is that they always require a relatively high order α of the differential operator in order to prove that the solution y possesses a large number of derivatives in the half-open interval $(0, T]$ or even in the closed interval $[0, h]$. However, it is also possible to obtain similar results if α is small if we impose stronger smoothness conditions on f. This follows from the next theorem.

Theorem 2.2.18. *Assume the hypotheses of Theorem 2.2.11. Moreover let $f \in C^k(G)$. Then $y \in C^k(0, T] \cap C^{n-1}[0, T]$, and for $l = n, n+1, ..., k$ we have $y^{(l)}(t) = O(t^{\alpha-l})$ as $t \to 0$.*

This theorem is a special case of ([23], Theorem 2.1). Thus, for the proof we refer to the original paper of Brunner et al. [23].

2.3 Mathematical modeling of infectious diseases

We now focus on how the mathematical models in the field of infectious diseases can be used to predict the future outcome of an epidemic process. Different forms of the (ordinary and fractional) differential equation models are given in the context of this section.

2.3.1 Historical background

Infectious diseases have ever been a great concern of human kind since the beginning of our history [166]. Infectious diseases are caused by pathogenic microorganisms, such as bacteria, viruses, parasites or fungi. The diseases can be spread, directly or indirectly, from one person to another or from animals to humans. The World Health Organization (WHO) reports that: Infectious diseases are responsible for a quarter to a third of all deaths in the world annually, the vast majority occurring in low-income and middle-income countries [175]. Even when infections do not kill, they reduce the quality of life for hundreds of millions of people and retard economic growth [92]. Population growth and spread, global climate change, and the emergence and reemergence of novel and deadly forms of infectious diseases have increased the need for sound quantitative methods to guide disease intervention practice [157]. In the last decades, influenza was pandemic several times and new diseases such as Lyme disease, Legionnaire's disease, toxic-shock syndrome, hepatitis C, hepatitis E, The human immunodeficiency virus (HIV), hantavirus were encountered [10] and recently the largest and most complex Ebola outbreak in West Africa, (first cases notified in March 2014) [55]. Millions died every year because of the infectious diseases. For example, the human immunodeficiency virus (HIV), which is the etiologic agent for acquired immunodeficiency syndrome (AIDS), was identified in 1981 and now causes over 3 million deaths per year in the world [176]. Another example of the most dangerous infectious diseases, the Hepatitis C. Hepatitis C (HCV) is a liver disease caused by the hepatitis C virus. Countries with high rates of chronic infection are Egypt (22%), Pakistan (4.8%) and China (3.2%). Most European countries report a prevalence of HCV in the general population of between 0.5 and 2%.

In the last few decades, mathematical models have become extremely important tools in

understanding, analyzing the spread and control of infectious diseases [26, 27, 35, 129]. Mathematical modeling of the spread of infectious diseases has become part of epidemiology policy decision-making in several countries, including the high income countries like United Kingdom, Netherlands, Canada, and the United States [85, 86]. Thus modeling approaches have become very important for decision-making about infectious disease intervention programs. Recent approaches include deterministic models, computer simulations, Markov Chain Monte Carlo models, small world and other network models, stochastic simulation models, and micro simulations of individuals in a community. These techniques are often implemented computationally and use data on disease incidence and population demographics. More specifically, since the eighteenth century, scientists have been using mathematical models of infectious diseases to inform public policy [85, 129, 166]. In 1766, [19] Bernoulli used smallpox mortality projections to argue for increased "inoculation", despite a lack of understanding of how the disease infected and killed people. In 1854, systematic observations led John Snow to identify a single water pump as the source of a cholera outbreak, thereby contributing to the development of epidemiology as a science (cf.[152]). By the beginning of the twentieth century, mathematical models had been developed for measles (Hamer, 1906 [82]) and malaria (Ross, 1910 [153]), and Kermack and McKendrick (1927 [88]) had established the mathematical theory of epidemics. The second half of the twentieth century saw further refinements in mathematical models for the invasion and persistence of human pathogens. Similar techniques were applied to the study of the spread of animal and plant diseases, both in agricultural and natural landscapes [129]. As a result, a theory emerged of how epidemics spread and how control measures should be deployed that can be applied to a wide range of pathogens, host populations, and environments.

2.3.2   What infectious diseases models can do?

In many sciences it is possible to conduct experiments to obtain information and test hypotheses. Experiments with the spread of infectious diseases in human [38] populations are often impossible, unethical or expensive. Data is sometimes available from naturally occurring epidemics or from the natural incidence of endemic diseases; however, the data is often incomplete due to underreporting. This lack of reliable data makes accurate parameter estimation difficult, so that it may only be possible to estimate a range of values for some parameters. Since repeatable experiments and accurate data are usually not available in epidemiology, mathematical models and computer simulations can be used to perform needed theoretical experiments. Calculations can easily be done for a variety of parameter values and data sets [4]. Optimal strategies for vaccination can be found theoretically by using modeling. The parameters used in an epidemiological model must have a clear interpretation such as a contact rate or duration of infection. Epidemiological models can sometimes be used to predict the spread or incidence of a disease. For example, Hethcote [85, 86] predicted that rubella and Congenital Rubella Syndrome will eventually disappear in the United States because the current vaccination levels using the combined measles-mumps-rubella vaccine are significantly above the threshold required for herd immunity for rubella. An epidemiological model can also be used to determine the sensitivity of predictions to changes in parameter values. After identifying the parameters which have the

greatest influence on the predictions, it may be possible to design studies to obtain better estimates of these parameters. An advantage of mathematical modeling of infectious diseases is the economy, clarity and precision of a mathematical formulation. Epidemiological modeling is an important part of the epidemiologist's function to build and test theories. Mathematical and computer simulation [9] models are the fundamental experimental tools in epidemiology. The only data usually available are from naturally occurring epidemics or from the natural incidence of endemic diseases; unfortunately, even these data are not complete since many cases are not reported. Since repeatable experiments and accurate data are usually not available in epidemiology, mathematical and computer simulation models must be used to perform necessary theoretical experiments with different parameter values and different data sets. It is easy in a computer simulation to find out what happens when one or several parameters are changed.

In general, we can conclude that epidemic modeling has three main aims. The first is to understand the spreading mechanism of the disease. For this, the essential part is a mathematical structure (equations give us threshold values and other constants which we use to describe the behavior of the disease). The second aim is to predict the future course of the epidemic. The third is to understand how we may control the spread of the epidemic.

2.3.3 The basic infectious diseases models

Mathematical infectious disease models are built from various components that represent the physical spread of the disease. Some of these components are the epidemiological compartment structure, the incidence rate form, the compartmental waiting time distributions, the population demographic structure, and the epidemiological-demographic interactions [94]. Because there are many choices for these various components, based on the situation being modelled, the combinatorial possibilities are enormous. Certainly, there are many modifications and extensions which depend critically on the disease being modelled and should be incorporated [21, 24, 68]. In classic deterministic epidemiological models, the population is split into different compartments which are assumed to be functions of discrete time $t = 0, 1, 2, ...$ or differentiable functions of continuous time $t \leq 0$. This enables us to derive sets of difference or differential equations governing the process. Only non-negative solutions for these system of equations are considered since negative solutions have no epidemiological significance. The choice of which compartments to use in the model depends on the characteristics of a particular disease and the purpose of the model. Compartments with labels such as M, S, E, I, and R are used for the epidemiological classes. If a pregnant woman is infected, her antibodies are transferred across placenta, so the new born infant has temporary passive immunity to that infection. The class M contains these infants with the passive immunity. When the infant looses his passive immunity, it enters the class of susceptible S, together with the infants who did not get the maternal immunity. This is the class of people who can get infected. So when there is an adequate contact of an infective individual (from class I) with a susceptible individual (from class S) and this individual gets infected, then this susceptible enters the class of exposed individuals E. These are the people in latent period who are infected but not yet infectious. When they become infectious (they are able to communicate the disease), then they enter class I- infectious. And finally, they enter the

class R- recovered. These are people with permanent immunity- which is acquired. Often, the disease models are named based on which compartments are used and the flow of individuals in these compartments, for example the classical models ([60, 178, 182]) like SI, SIS, SIR, SIRS, MSEIR, MSEIRS, SEIR, SEIRS, SEI and SEIS models. Now, we will introduce some of these models as follow:

The SIR epidemic model:

Epidemic models has been widely used in different forms for studying epidemiological processes such as the spread of influenza and SARS and even for the spread of rumors [15, 128]. The research results are helpful to predict the developing tendency of the infectious disease, to determine the key factors of the spread of infectious disease and to seek the optimum strategies of preventing and controlling the spread of infectious diseases. In contrast with classic biometrics, dynamical methods can show the transmission rules of infectious diseases from the mechanism of transmission of the disease, so that people may know some global dynamic behavior of the transmission process. Combining statistics methods and computer simulations with dynamic methods could make modeling and the original analysis more realistic and more reliable; make the comprehension for spread rule of infectious diseases more thorough. Now, the popular epidemic dynamic models are still so called a compartmental model which were constructed by Kermack and Mckendrick [88] in 1927 and is developed by many other bio-mathematicians [15]. In this model which is called SIR model, the population is divided into three compartments: susceptible compartment S, in which all individuals are susceptible to the disease; infected compartment I, in which all individuals are infected by the disease and have infectivity; removed compartment R, in which all the individuals recovered from the class I and have permanent immunity. The SIR epidemic model can be written as:

$$\frac{dS}{dt} = -\beta SI,$$

$$\frac{dI}{dt} = \beta SI - \gamma I,$$

$$\frac{dR}{dt} = \gamma I.$$

Where $S(t)$, $I(t)$, and $R(t)$ are the numbers in these classes, so that

$$S(t) + I(t) + R(t) = N, \ S(0) = S_0 \geq 0, \ I(0) = I_0 \geq 0, \ R(0) = R_0 \geq 0.$$

This SIR model is a special case of the model MSEIR [129], in which the passively immune class M and the exposed class E are omitted. This model uses the standard incidence and has recovery at rate γI, corresponding to an exponential waiting time $e^{-\gamma I}$. The constant β is defined as the contact rate. This model has no vital dynamics (births and deaths).

The SIR endemic model:

The classic endemic model is the SIR model with vital dynamics given by

$$\frac{dS}{dt} = \mu N - \mu S - \frac{\beta SI}{N},$$

$$\frac{dI}{dt} = \frac{\beta SI}{N} - \gamma I - \mu I,$$

$$\frac{dR}{dt} = \gamma I - \mu R.$$

Where

$$S(t) + I(t) + R(t) = N, \ S(0) = S_0 \geq 0, \ I(0) = I_0 \geq 0, \ R(0) = R_0 \geq 0.$$

This SIR model is almost the same as the SIR epidemic model above, except that it has an inflow of newborns into the susceptible class at rate μN and deaths in the classes at rates μS, μI, and μR [86]. The deaths balance the births, so that the population size N is constant.

2.3.4 The basic reproduction number

One of the main goals of studying epidemiology models is to analyze the spread of a disease in order to try to understand its underlying principles. The reason for this is to be able to come to some conclusions about the severity and duration of the epidemic. Certainly, it is desired to be able to answer important questions such as: Will there be an epidemic? If so, how long will it last? How severe might it be? Can the disease be eradicated through some type of control scheme?

Thresholds that dictate the persistence or eradication of a disease are very important in epidemiology [128]. Hence, one of the main goals of disease modelling is to establish criteria based on the parameters and structure of the system that will ensure disease eradication. The often used the threshold number is the basic reproduction number $\mathcal{R}_0$. It is defined as the average number of secondary infections produced by one infected individual in a wholly susceptible population. According to this meaning, it is easy to understand that if $\mathcal{R}_0 < 1$ then the infectives will decrease so that the disease will go to extinction; if $\mathcal{R}_0 \geq 1$ then the infectives will increase so that the disease cannot be eliminated and usually develop into an endemic.

2.3.5 Fractional order models of infectious diseases

To start again with the preface of Mathematical epidemiology: "The mathematics is dictated by the epidemiology and not vice versa". Sometimes, we need to explore new methods or find new ways in order to make biological models more realistic. In today's epidemiology problems, it may be advantageous to use fractional calculus in existing models. The fractional order can be introduced to any one of the presented models. FODEs are at least as stable as their integer order counterparts. This is because systems with memory are typically more stable than their

memory-less alternatives [58]. FDEs are naturally related to systems with memory which exists in most biological systems. Also, they are closely related to fractals [59, 110], which are abundant in biological systems. Although a large number of researches have been done on modeling the dynamics of many infectious diseases, it has been restricted to integer order (delay) differential equations. Recently, many researchers have tried to model real processes using the fractional calculus. The fractional calculus may be considered an old and yet novel topic. In [3], the authors studied a FDE model which describes the spread of Hantavirus infection in a system consisting of the host species and a non-host competitor species. Demirci et al. [37] introduce the fractional order SEIR model with vertical transmission in a population with density dependent death rate. In [6] a fractional order model for nonlocal epidemics was studied. The obtained results in [6] were expected to be relevant to foot-and-mouth disease, SARS and avian flu. In [163], an approximate solution of a fractional order differential system for modeling human T-cell lymphotropic virus I (HTLV- I) infection of $CD4^+$T-cells was presented. In [7] E. Ahmed et al. presented a fractional order generalization of basic hepatitis C virus (HCV) model including an immune response term. The authors in [52] presented a fractional order model of the infection of HIV-1. The authors in [144] introduced the use of fractional calculus, i.e., the use of integrals and derivatives of non-integer (arbitrary) order, in epidemiology and they succeeded to find the best value of fractional order α that makes the model more realistic.

Chapter 3

Numerical methods for FODEs

In this chapter, we focus on introducing numerical methods for FODEs of Caputo-type. We can note that there are several ways to discretize FODE of Caputo-type; the most often used two techniques are based on the following ideas:

- Discretizing the Caputo derivative directly to get the numerical schemes.

- Transforming the original fractional equation into the fractional integral equation, then applying the corresponding numerical methods to discretize the fractional integral to get the numerical schemes.

3.1   Fractional linear multistep methods

The fractional linear multistep method (FLMM) for fractional calculus was first studied by Lubich [113, 114, 117], which can be seen as the generalization of the linear multistep method (LMM) for classical calculus (see Lemma 1.1.23). In this section, we introduce the FLMMs for fractional order integral based on the definition and theorems in article [113]. Then, we can conclude the FLMMs for the FODE of Caputo-type and investigate its properties (consistent, convergence and stability). We now remind ourselves that in case of a linear multistep method we are interested in a solution y on a closed interval $[0, X]$ for some $X > 0$ and that we seek a solution on a prescribed set of nodes in this interval. These nodes are arranged equispaced inside the interval $[0, X]$ and on its border with a given step-size h and are additionally assumed to be numbered increasingly $x_0, x_1, ..., x_N$, where $N = X/h$, $x_0 = 0$ and $x_N = X$.

Definition 3.1.1. Let $f : [0, X] \to \mathbb{C}$. An approximation to the integral equation

$$y(x) = (I^\alpha f)(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x - s)^{\alpha-1} f(s) ds, \quad x \in [0, X] \tag{3.1}$$

given by

$$(_h I^\alpha f)(x_n) = h^\alpha \sum_{j=0}^n \omega_{n-j} f(jh) + h^\alpha \sum_{j=0}^s w_{nj} f(jh), \quad n = 0, 1, .., N \tag{3.2}$$

with some fixed $s \in \mathbb{N}$ is called fractional convolution quadrature ω. The weights ω_j are called convolution weights and the term

$$_h\Omega^\alpha f(x) := h^\alpha \sum_{j=0}^{n} \omega_{n-j} f(jh), \quad x = nh \tag{3.3}$$

is called convolution part with corresponding convolution quadrature error given by

$$_hE^\alpha = {}_h\Omega^\alpha - I^\alpha.$$

The term

$$_hS^\alpha f(x) := h^\alpha \sum_{j=0}^{s} w_{nj} f(jh),$$

is called starting part and the weights w_{nj} starting weights.

In the following results we extend the concepts of Definition 1.1.25 to inculed fractional convolution quadrature ω. Again $\omega(\zeta)$ denotes the generating function of the convolution weights ω_j as in Lemma 1.1.23 :

Definition 3.1.2.   1. A fractional convolution quadrature is stable (for I^α) if

$$\omega_n = O(n^{\alpha-1}).$$

2. A fractional convolution quadrature is consistent of order p (for I^α) if

$$h^\alpha \omega(e^{-h}) = 1 + O(h^p).$$

3. A fractional convolution quadrature is convergent of order p (to I^α) if

$$(_hE^\alpha x^{z-1})(1) = O(h^z) + O(h^p), \tag{3.4}$$

holds for all $z \in \mathbb{C}\backslash\{0, -1, -2, ...\}$.

Remark 3.1.3. **a)** For $\alpha > 0$, the condition for consistency can also be interpreted as

$$h^\alpha \sum_{j=0}^{\infty} \omega_j e^{-jh} = \frac{1}{\Gamma(\alpha)} \int_0^\infty t^{\alpha-1} e^{-t} dt + O(h^p),$$

i.e. the convolution part of the fractional convolution quadrature yields an $O(h^p)$ approximation to the integral of the exponential function on the interval $(0, \infty)$.

b) The standardization at the point $x = 1$ in equation (3.4) is justified by

$$(_hE^\alpha t^{z-1})(x) = x^{\alpha+z-1}(_{h/x}E^\alpha t^{z-1})(1), \quad x > 0, \tag{3.5}$$

which can be deduced as follows: for $x > 0$ we have

$$I^\alpha x^{z-1} = \frac{\Gamma(z)}{\Gamma(z+\alpha)}x^{z-1+\alpha} \quad \text{and} \quad _h\Omega^\alpha x^{z-1} = n^{-\alpha}\sum_{j=0}^n \omega_{n-j}\left(\frac{j}{n}\right)^{z-1}x^{z-1+\alpha} \quad (x = nh).$$

Thus,

$$
\begin{aligned}
_hE^\alpha(t^{z-1})(x) &= x^{z-1+\alpha}\left(n^{-\alpha}\sum_{j=0}^n \omega_{n-j}\left(\frac{j}{h}\right)^{z-1} - \frac{\Gamma(z)}{\Gamma(z+\alpha)}\right) \\
&= x^{\alpha+z-1}(_{h/x}E^\alpha t^{z-1})(1).
\end{aligned}
$$

We now consider a fractional convolution quadrature ω for which

$$\omega(\zeta) = (r_1(\zeta))^\alpha (r_2(\zeta)), \tag{3.6}$$

where $r_i(\zeta)$ are rational functions and α be a non-integer number, then we have the main result of this section.

Theorem 3.1.4. *A fractional convolution quadrature (3.6) is convergent of order p if and only if it is stable and consistent of order p.*

Proof. We will break the proof into several steps which are formulate as Lemmas. Lemma 3.1.6 will prove that convergence of order p implies consistency of order p, Lemma 3.1.9 will show that stability also follows from convergence and finally in Lemma 3.1.13 we will see that stability and consistency of order p imply convergence of order p of a fractional convolution quadrature. We also need some preparations to prove these three Lemmas. $\qquad\square$

Lemma 3.1.5. *Let $\alpha > 0$ and f, g be two continuous functions. Then*

$$_hE^\alpha(f * g) = {}_hE^\alpha f * g, \tag{3.7}$$

where $*$ denotes the Laplace convolution (see Definition 1.2.4).

Proof. From Definition 2.1.1, we have

$$(I^\alpha f)(x) = \left(\frac{x^{\alpha-1}}{\Gamma(\alpha)} * f\right)(x)$$

by the associativity of the convolution operator

$$I^\alpha(f * g) = \frac{x^{\alpha-1}}{\Gamma(\alpha)}(f * g) = \left(\frac{x^{\alpha-1}}{\Gamma(\alpha)} * f\right) * g = (I^\alpha f) * g,$$

holds for the given functions f and g. $_h\Omega^\alpha f(x_n)$, introduced in (3.3), can be written as follow

$$_h\Omega^\alpha f(x_n) = h^\alpha \sum_{j=0}^{n} \omega_j f(x_n - x_j),$$

we find that

$$
\begin{aligned}
(_h\Omega^\alpha(f * g))(x_n) &= h^\alpha \sum_{j=0}^{n} \omega_j (f * g)(x_n - x_j) \\
&= h^\alpha \sum_{j=0}^{n} \omega_j \int_0^{x_n - x_j} f(s)g(x_n - x_j - s)ds \\
&= h^\alpha \sum_{j=0}^{n-1} \omega_j \int_0^{x_n - x_j} f(s)g(x_n - x_j - s)ds, \qquad (3.8)
\end{aligned}
$$

where we used in the last step that

$$\lim_{x \to 0}(f * g)(x) = 0.$$

Furthermore,

$$
\begin{aligned}
(_h\Omega^\alpha f * g)(x_n) &= \int_0^{x_n} (_h\Omega^\alpha f)(t)g(x_n - t)dt \\
&= h^\alpha \int_0^{x_n} \sum_{0 \le x_j \le t} \omega_j f(t - x_j)g(x_n - t)dt \\
&= h^\alpha \sum_{k=0}^{n-1} \int_{x_k}^{x_{k+1}} \sum_{0 \le x_j \le t} \omega_j f(t - x_j)g(x_n - t)dt \\
&= h^\alpha \sum_{k=0}^{n-1} \sum_{j=0}^{k} \omega_j \int_{x_k}^{x_{k+1}} f(t - x_j)g(x_n - t)dt \\
&= h^\alpha \sum_{j=0}^{n-1} \omega_j \sum_{k=j}^{n-1} \int_{x_k}^{x_{k+1}} f(t - x_j)g(x_n - t)dt \\
&= h^\alpha \sum_{j=0}^{n-1} \omega_j \int_{x_j}^{x_n} f(t - x_j)g(x_n - t)dt \\
&= h^\alpha \sum_{j=0}^{n-1} \omega_j \int_0^{x_n - x_j} f(s)g(x_n - x_j - s)ds.
\end{aligned}
$$

By (3.8), we have

$$(_h\Omega^\alpha f * g)(x_n) = (_h\Omega^\alpha(f * g))(x_n).$$

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This implies that,

$$
\begin{aligned}
{}_hE^\alpha(f * g) &= {}_h\Omega^\alpha(f * g) - I^\alpha(f * g) \\
&= {}_h\Omega^\alpha f * g - I^\alpha f * g = {}_hE^\alpha f * g.
\end{aligned}
$$

$\square$

Lemma 3.1.6. *Let $\alpha > 0$ and ${}_hE^\alpha x^{k-1} = O(h^k) + O(h^p)$ for $k = 1, 2, 3, ...$, then the fractional convolution quadrature ω is consistent of order p. In particular, convergence of order p implies consistency of order p.*

Proof. By Definition 3.1.2 for consistency of order p we need to show that $h^\alpha \omega(e^{-h}) = 1 + O(h^p)$. We will first prove that $\lim_{x \to \infty} e_h(x) = h^\alpha \omega(e^{-h}) - 1$ holds for an auxiliary function $e_h(x)$ and afterwards that $\lim_{x \to \infty} e_h(x) = O(h^p)$ holds, which will thus conclude our proof.

Let $u(t) = e^{t-x}$ be a function defined on the interval $[0, x]$. Then the convolution quadrature error of this function is given by

$$
e_h(x) := ({}_hE^\alpha e^{t-x})(x) = h^\alpha \sum_{0 \le jh \le x} \omega_j e^{-jh} - \frac{1}{\Gamma(\alpha)} \int_0^x s^{\alpha-1} e^{-s} ds.
$$

Taking the limit $x \to \infty$ we get

$$
\lim_{x \to \infty} e_h(x) = h^\alpha \omega(e^{-h}) - 1. \tag{3.9}
$$

We expand e^{t-x} at $t = 0$,

$$
e^{t-x} = e^{-x} \sum_{j=0}^{m-1} \frac{t^j}{j!} + \frac{1}{(m-1)!}(s^{m-1} * e^{s-x})(t); \quad m \in \mathbb{N}.
$$

Therefore, we can write

$$
e_h(x) = e_h^1(x) + e_h^2(x),
$$

with

$$
e_h^1(x) := e^{-x} \sum_{j=0}^{m-1} \frac{1}{j!}({}_hE^\alpha t^j)(x) \quad \text{and} \quad e_h^2(x) := \frac{{}_hE^\alpha(t^{m-1} * e^{t-x})(x)}{(m-1)!}.
$$

By (3.5), $({}_hE^\alpha t^j)(x)$ has only polynomial growth as $x \to \infty$. Hance

$$
\lim_{x \to \infty} e_h^1 = 0.
$$

From result (3.7) of Lemma 3.1.5 follows:

$$
(m-1)! \, e_h^2(t) = {}_hE^\alpha(t^{m-1} * e^{t-x})(x) = ({}_hE^\alpha t^{m-1} * e^{t-x})(x) = \int_0^x e^{-s}({}_hE^\alpha t^{m-1})(s) ds.
$$

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So we have the limit $x \to \infty$ as follows

$$\lim_{x \to \infty} e_h^2 = \frac{1}{(m-1)!} \int_0^\infty e^{-s} (_h E^\alpha t^{m-1})(s) ds.$$

By (3.5) and the assumptions follows (with sufficiently large m, i.e. $m \geq p$) that

$$(_h E^\alpha t^{m-1})(s) = s^{\alpha+m-1} (_{h/s} E^\alpha t^{m-1})(1) = O(s^{\alpha-1} h^p),$$

and thus

$$\lim_{x \to \infty} e_h^1(x) = O(h^p), \quad h \to 0.$$

i.e. consistency of order p. □

Now, we may write the function $\omega(\zeta)$ (3.6) as

$$\omega(\zeta) = (1-\zeta)^{-\mu} \tilde{\omega}(\zeta), \tag{3.10}$$

where μ is chosen such that $\tilde{\omega}(\zeta)$ is analytic at 1 and $\tilde{\omega}(1) \neq 0$. Consistency implies immediately $\mu = \alpha$ and $\tilde{\omega}(1) = 1$. Expanding ω at 1 yields:

$$\omega(\zeta) = (1-\zeta)^{-\alpha} \left[c_0 + c_1(1-\zeta) - c_2(1-\zeta)^2 + \ldots + c_{N-1}(1-\zeta)^{N-1} \right] + (1-\zeta)^N r(\zeta), \tag{3.11}$$

where $r(\zeta) := (1-\zeta)^{-\alpha} \tilde{r}(\zeta)$ and $\tilde{r}(\zeta)$ is analytic at 1. Thus, we can now characterize consistency in the terms of the coefficients c_j in (3.11).

Lemma 3.1.7. *Let γ_j denote the coefficients of*

$$\sum_{j=0}^\infty \gamma_j (1-\zeta)^j = \left(\frac{-\ln \zeta}{(1-\zeta)} \right)^{-\alpha}.$$

Then the fractional convolution quadrature ω is consistent of order p if and only if the coefficients c_j in (3.11) satisfy $c_j = \gamma_j$ for $j = 0, 1, ..., p-1$.

Proof. For consistency of order p we need to show that $h^\alpha \omega(e^{-h}) = 1 + O(h^p)$. From (3.10) follows

$$h^\alpha \omega(e^{-h}) = \left(\frac{h}{1-e^{-h}} \right)^\alpha \tilde{\omega}(e^{-h}),$$

which satisfies $1 + O(h^p)$ if and only if

$$\tilde{\omega}(e^{-h}) = \left(\frac{h}{1-e^{-h}} \right)^{-\alpha} + O(h^p).$$

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(in the above equation $O(h^{p-\alpha})$ would have been sufficient, but analyticity of $\tilde\omega$ implies $O(h^p)$).
This holds if and only if

$$\tilde\omega(\zeta) = \left(\frac{-\ln\zeta}{1-\zeta}\right)^{-\alpha} + O((1-\zeta)^p).$$

$\square$

In the following lemma we will use the fact that the binomial coefficients possess the asymptotic expansion:

$$(-1)^n\binom{-\alpha}{n} = \frac{n^{\alpha-1}}{\Gamma(\alpha)}[1 + a_1n^{-1} + ... + a_{N-1}n^{-N+1} + O(n^{-N})], \tag{3.12}$$

where the coefficients a_j depend analytically on α (see e.g [170]). With this result we can point out in which way the stability of a fractional convolution equation ω depends on the remainder of the expression (3.11):

Lemma 3.1.8. *The fractional convolution quadrature ω is stable if and only if the coefficients r_n of $r(\zeta)$ in (3.11) satisfy*

$$r_n = O(n^{\alpha-1}). \tag{3.13}$$

Proof. Let $r_n = O(n^{\alpha-1})$. For stability we have to show that $\omega_n = O(n^{\alpha-1})$ (from Definition 3.1.2). The convolution weights are given in equation (3.11) as

$$\omega_n = \sum_{j=0}^{N-1}(-1)^n\binom{-\alpha+j}{n}c_j + \sum_{k=0}^{n}(-1)^k\binom{-\alpha+N}{k}r_{n-k}.$$

Thus by (3.12) it follows that $\omega_n = O(n^{\alpha-1})$.

Conversely, let ω be stable. Then $\omega(\zeta)$ has no singularities in the interior of the unit disc and by(3.6) can be written as

$$\omega(\zeta) = u(\zeta)\left((\zeta-1)^{-\alpha} - \prod_{j=0}^{m}(\zeta-\zeta_j)^{-\alpha_j}\right), \tag{3.14}$$

where

$$|\zeta_j| = 1, \ u(\zeta) \neq 0, \ \alpha_j > 0, \ \zeta_i \neq \zeta_j \text{ for } i,j = 1,2,...,m$$

and $u(\zeta)$ is analytic in a neighbourhood of $|\zeta| \leq 1$. A partial fraction decomposition of $\omega(\zeta)$ yields

$$\omega(\zeta) = (\zeta-1)^{-\alpha}u(\zeta) + \sum_{j=0}^{m}(\zeta-\zeta_j)^{-\alpha_j}p_j(\zeta-\zeta_j) + q(\zeta),$$

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where the p_j are polynomials satisfying $p_j(0) = 0$ and $q(\zeta)$ is analytic in the interior of the unit disc and sufficiently differentiable on the unit circle $|\zeta| = 1$. From (3.12) follows

$$\omega_n = O(n^{\alpha-1}) \Leftrightarrow \alpha_j \le \alpha, \ j = 1, ..., m. \tag{3.15}$$

Correspondingly, $r(\zeta)$ can be represented as

$$r(\zeta) = (\zeta - 1)^{-\alpha}\tilde{u}(\zeta) + \sum_{j=0}^{m}(\zeta - \zeta_j)^{-\alpha}\tilde{p}_j(\zeta - \zeta_j) + \tilde{q}(\zeta),$$

with $\tilde{u}, \tilde{p}_j$ and $\tilde{q}$ are linked to $\tilde{\omega}$ as u, p_j and q to ω. Thus $r_n = O(n^{\alpha-1})$ holds. □

Lemma 3.1.9. *The fractional convolution quadrature ω is stable of order p if it is convergent of order p.*

Proof. From Definition 3.1.2, convergence of ω implies $({}_hE^\alpha x^{z-1})(1) = O(h^z) + O(h^p)$. By Lemma 3.1.6 this implies also consistency of ω. We can therefore write $\omega(\zeta)$ with $N = 1$ in (3.11) as

$$\omega(\zeta) = (1 - \zeta)^{-\alpha} + (1 - \zeta)r(\zeta) \Rightarrow \frac{\omega(\zeta)}{1 - \zeta} = (1 - \zeta)^{-\alpha-1} + r(\zeta),$$

and thus

$$(-1)^n\binom{-\alpha-1}{n} + r_n$$

is the nth coefficient of $\omega(\zeta)/(1 - \zeta)$. On the other hand

$$\frac{\omega(\zeta)}{1 - \zeta} = \omega(\zeta)\frac{1}{1 - \zeta} = \left(\sum_{j=0}^{\infty}\omega_j\zeta^j\right)\left(\sum_{k=0}^{\infty}\zeta^k\right)$$

$$= \sum_{j=0}^{\infty}\sum_{k=0}^{j}\omega_{j-k}\zeta^j.$$

Therefore, we can conclude

$$\sum_{k=0}^{n}\omega_{n-k} = (-1)^n\binom{-\alpha-1}{n} + r_n.$$

Now, we consider the convolution quadrature error

$$({}_hE^\alpha 1)(1) = h^\alpha\sum_{j=0}^{n}\omega_{n-j} - \frac{1}{\Gamma(\alpha+1)}, \quad (nh = 1)$$

$$= h^\alpha\left[(-1)^n\binom{-\alpha-1}{n}\right] + h^\alpha r_n - \frac{1}{\Gamma(\alpha+1)}.$$

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With (3.12) follows

$$
\begin{aligned}
(_hE^\alpha 1)(1) &= h^\alpha \left[\frac{n^\alpha}{\Gamma(\alpha+1)} + O(n^{\alpha-1}) \right] + h^\alpha r_n - \frac{1}{\Gamma(\alpha+1)} \\
&= O(h) + h^\alpha r_n.
\end{aligned}
$$

Thus $(_hE^\alpha 1)(1) = O(h) \Leftrightarrow r_n = O(n^{\alpha-1})$. □

To arrive at the final step of the proof, we need to state an auxiliary results on the structure of the error of the fractional convolution quadrature ω. A proof of this lemmas can be found e.g. in ([113], Lemma 3.5, Lemma 3.6 and Lemma 3.7).

Lemma 3.1.10. *Let $\alpha, z > 0$ and the fractional convolution quadrature ω be stable. Then the convolution quadrature error of t^{z-1} has an asymptotic expansion of the form*

$$
(_hE^\alpha t^{z-1})(1) = e_0 + e_1 h + ... + e_{N-1} h^{N-1} + O(h^N) + O(h^z). \tag{3.16}
$$

where the coefficients e_j depend analytically on α, z.

Lemma 3.1.11. *Let $\alpha > 0$ and $(_hE^\alpha t^{p-1})(1) = O(h^p)$. Then*

$$
(_hE^\alpha t^{q-1})(1) = O(h^p), \text{ for all } q > p.
$$

Lemma 3.1.12. *Let $\alpha > 0$ and let ω be a stable fractional convolution quadrature. Then there exist numbers $\gamma_0, \gamma_1, \gamma_2, ...$ independent of the generating function $\omega(\zeta)$ such that the following equivalence holds:*

$$
(_hE^\alpha t^{q-1})(1) = O(h^q) \text{ for } q = 1, 2, ..., p \tag{3.17}
$$

if and only if the coefficients c_i in (3.11) satisfy

$$
c_i = \gamma_i \text{ for } i = 0, 1, 2, ..., p-1.
$$

With the following Lemma we have successfuly proven Theorem 3.1.4.

Lemma 3.1.13. *Let $\alpha > 0$. If the fractional convolution quadrature ω be stable and consistent of order p, then ω is convergent of order p.*

Proof. First we note that the numbers γ_i of Lemma 3.1.12 and Lemma 3.1.7 are identical since ω is assumed to be consistent. Moreover, because of the stability of ω we get from Lemma 3.1.10 and Lemma 3.1.11 for $z > p$

$$
e_k(\alpha, z, \gamma_0, ..., \gamma_j) = 0, \quad k = 0, ..., p-1.
$$

At last, by Lemma 3.1.7 consistency of order p implies

$$
e_i = \gamma_i \quad i = 0, ..., p-1,
$$

so that

$$
(_hE^\alpha x^{z-1})(1) = O(h^z) + O(h^p)
$$

holds for all $z \in \mathbb{C} \backslash \{0, -1, -2, ...\}$ and thus ω is convergent of order p. □

If $\alpha = 1$ in the fractional convolution quadrature (3.6) we have in essence reproduced Dahlquist's convergence theorem for linear multistep methods [32, 33].

In [34] there is another important result, if we take $(_hIf)(x)$ as solution of a linear multistep method (σ, ρ) applied to the problem $y' = f$, $y(0) = 0$ as described in Lemma 1.1.23, then the repeated method $(_hI^kf)(x) = (_hI..._hIf)(x)$, $k \in \mathbb{N}$ can be written as a convolution quadrature, where the convolution weights ω_n are the coefficients of the generating function $\omega(\zeta)^k$, with $\omega(\zeta)$ given by (1.8). This method can be interpreted as kth power of the multistep method. Now we want to transfer this idea to fractional case. For this purpose the following theorem show the αth power of a linear multistep method, with $\alpha \in \mathbb{R}$.

Theorem 3.1.14. *(**fractional linear multistep methods**) Let (σ, ρ) denote an implicit classical linear multistep method which is stable and consistent of order p and assume that all zeros of $\sigma(\zeta)$ lie inside or on the unit disc. Furthermore, let ω be the generating function of the linear multistep method. If we define the generating function $\omega^\alpha(\zeta)$ by*

$$\omega^\alpha(\zeta) = (\omega(\zeta))^\alpha. \tag{3.18}$$

Then the fractional convolution quadrature ω^α is convergent of order p to I^α.

Proof. Because of Theorem 3.1.4 we only need to show that ω^α is consistent and stable. For consistency, we known that the linear multistep method is consistent of order p, i.e.

$$h\omega(e^{-h}) = 1 + O(h^p).$$

Taking this relation to the power α yields

$$h^\alpha \omega^\alpha(e^{-h}) = 1 + O(h^p),$$

so that ω^α is consistent of order p to I^α. To prove stability of the method, we note that under the given assumptions on (σ, ρ) we can write

$$\omega(\zeta) = \frac{\sigma(\zeta^{-1})}{\rho(\zeta^{-1})} = \prod_{j=0}^{r}(1 - \zeta_j\zeta)^{-1}v(\zeta),$$

where $v(\zeta)$ is analytic and without zeros in a neighbourhood of $|\zeta| \leq 1$, and ζ_j are the zeros of $\rho(\zeta)$ on the unit circle. Thus

$$\omega^\alpha(\zeta) = \prod_{j=0}^{r}(1 - \zeta_j\zeta)^{-\alpha}u(\zeta),$$

where $u(\zeta) = v(\zeta)^\alpha$ is analytic in a neighbourhood of $|\zeta| \leq 1$. By (3.14) and (3.15) we get

$$\omega_n^\alpha = O(n^{\alpha-1})$$

so that ω^α is stable. $\qquad\square$

As seen in Definiton 3.1.2 the stability, consistency and convergence of a fractional convolution quadrature were defined without the use of the starting part in (3.2). If we consider a fractional convolution quadrature as defined in (3.2), which converges with order p to I^α, we will always be able to find a set of starting weights, so that for a sufficiently well behaved function f the fractional convolution quadrature error, i.e. $_hI^\alpha f - I^\alpha f$, is also of order p. Consequently, the following two theorems, can be found in [135], define what we understand under a sufficiently well behaved function f and show how we obtain the set of starting weights. They are generalizations of Theorem 2.4 in [113] and Theorem 6.1.4 in [22].

Theorem 3.1.15. *Let (σ, ρ) be a convergent implicit linear multistep method of order $p \geq 1$ and let all zeros of $\sigma(\zeta)$ lie inside or on the unit disc and*

$$\omega^\alpha(\zeta) = \left(\frac{\sigma(1/\zeta)}{\rho(1/\zeta)} \right)^\alpha, \quad \alpha > 0.$$

Furthermore, let

$$f(x) := \sum_{j=0}^{L} x^{z_j} v_j(x), \quad 0 \leq z_j \leq p - 1, \ v_j \in C^p[0, X], \ j = 0, 1, ..., L \tag{3.19}$$

and

$$A_j := \{\gamma = k + z_j | k \in \mathbb{N}_0, \ \gamma \leq p - 1\}, \quad A := \bigcup_{j=0}^{L} A_j, \tag{3.20}$$

and $s_j := \mathrm{card} A_j - 1$, $s := \mathrm{card} A - 1$. If we define the starting weights w_{nj} by the linear system

$$\sum_{j=0}^{s} w_{nj} j^\gamma = \frac{\Gamma(\gamma + 1)}{\Gamma(\gamma + \alpha + 1)} n^{\gamma + \alpha} - \sum_{j=0}^{n} \omega_{n-j} j^\gamma, \quad \gamma \in A, \tag{3.21}$$

then the following statements hold:

1. *$w_{nj} = O(n^{\alpha - 1}), \quad j = 0, ..., s,$*

2. *$_hI^\alpha f(x) - I^\alpha f(x) = O(h^{p - \varepsilon})$, with some $0 \leq \varepsilon < 1$ uniformly for all fixed $x_n = nh := x \in [0, X]$.*

The next theorem states a result on the set of starting weights, to be approximated by a fractional convolution quadrature, if the function $f(x)$ possesses a singularity at the origin.

Theorem 3.1.16. *Let (σ, ρ) be a convergent implicit linear multistep method of order $p \geq 1$ and let all zeros of $\sigma(\zeta)$ lie inside or on the unit disc and*

$$\omega^\alpha(\zeta) = \left(\frac{\sigma(1/\zeta)}{\rho(1/\zeta)} \right)^\alpha, \quad \alpha > 0.$$

Furthermore, let

$$f(x) := \sum_{j=0}^{L} x^{r_j-1} v_j(x), \quad 0 \le r_j \le p, \ v_j \in C^p[0,X], \ j = 0,1,...,L \tag{3.22}$$

and

$$A_j := \{\gamma = k + r_j | k \in \mathbb{N}_0, \ \gamma \le p\}, \quad A := \bigcup_{j=0}^{L} A_j, \tag{3.23}$$

and $s_j := \mathrm{card} A_j - 1$, $s := \mathrm{card} A - 1$. If we define the starting weights w_{nj} by the linear system

$$\sum_{j=0}^{s} w_{nj} j^{\gamma} = \frac{\Gamma(\gamma)}{\Gamma(\gamma+\alpha)} n^{\gamma+\alpha+1} - \sum_{j=0}^{n} \omega_{n-j} j^{\gamma-1}, \quad \gamma \in A, \tag{3.24}$$

then the following statements hold:

1. *$w_{nj} = O(n^{\alpha-1}), \quad j = 0,...,s,$*

2. *$_h I^{\alpha} f(x) - I^{\alpha} f(x) = O(h^{p-\varepsilon})$, with some $0 \le \varepsilon < 1$ uniformly for all fixed $x_n = nh := x \in [0,X]$.*

The last results stated that we will always find a set of starting weights so that the error of the fractional convolution quadrature behaves as it does in the case of classical convolution quadratures.

We are now going to extend Theorem 3.1.15 to Volterra-Abel integral equations of the second kind, i.e. we will be interested in convolution quadrature for equations of the form (see also Definition 2.2.6)

$$y(x) = g(x) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} K(x,t,y(t)) dt, \quad x \in [0,X], \ \alpha > 0 \tag{3.25}$$

where the kernel $K(x,t,y(t))$ is a bounded (and usually smooth) function. From Lemma 2.2.3 we know that fractional order differential equations can be transferred to Volterra integral equations of the form (3.25), where the function $g(x)$ is defined by the initial condition(s) and the kernel K is the right-hand side of the fractional order differential equation. Thus by construction a fractional convolution quadrature for the equation (3.25) will give results for fractional order differential equations as well. The following results are based on an article by Lubich [114]:

From Corollary 3 in [115] we know that the solution $y(x)$ is unique on a nonempty existance interval (assumed to contain the whole interval $[0,X]$). Thus, we can state the following result:

Theorem 3.1.17. *Let (σ, ρ) be a convergent implicit linear multistep method of order $p \ge 1$ and let all zeros of $\sigma(\zeta)$ lie inside or on the unit disc and*

$$\omega^{\alpha}(\zeta) = \left(\frac{\sigma(1/\zeta)}{\rho(1/\zeta)}\right)^{\alpha}, \quad 0 < \alpha < 1.$$

Furthermore, set

$$A = \{\gamma = k + j\alpha; \; k, j \in \mathbb{N}_0, \; \gamma \leq p - 1\}, \; cardA = s + 1 \qquad (3.26)$$

and define

$$y_n = g(x_n) + h^\alpha \sum_{j=0}^{n} \omega_{n-j} K(x_n, x_j, y(x_j)) + h^\alpha \sum_{j=0}^{s} w_{n,j} K(x_n, x_j, y(x_j)) \qquad (3.27)$$

as discretization of the Volterra-Abel integral equation (3.25), where the convolution weights ω_k are given by the generating function $\omega^\alpha(\zeta)$ and the starting weights are constructed by the linear equation system

$$\sum_{j=0}^{s} w_{n,j} j^\gamma = \frac{\Gamma(\gamma + 1)}{\Gamma(\gamma + \alpha + 1)} n^{\gamma + \alpha} - \sum_{j=1}^{n} \omega_{n-j} j^\gamma, \quad \gamma \in A. \qquad (3.28)$$

Then $w_{n,j} = O(n^{\alpha-1})$ and the numerical solution y_n satisfies

$$\max_{0 \leq n \leq N} |y_n - y(x_n)| = O(h^{p-\epsilon}), \qquad (3.29)$$

with some $0 \leq \epsilon < 1 - \alpha$. In particular $\epsilon = 0$ if $\alpha = q/(q+1)$ with $q \in \mathbb{N}$.

Proof. A proof of this theorem is given in [114] using discretized operational calculus [116]. $\qquad \square$

3.2 Fractional backward difference methods

In this section we want to develop numerical algorithms for the solution of the fractional order differential equation of Caputo type

$$^C D^\alpha y(x) = f(x, y(x)), \quad D^k y(0) = y_0^{(k)} \quad (k = 0, 1, ..., n - 1), \qquad (3.30)$$

where $\alpha > 0$, $\alpha \notin \mathbb{N}$ and $n = \lceil \alpha \rceil$. We are interested in a solution $y(x)$ for equation (3.30) on a closed interval $[0, X]$ for some $X > 0$. As in the classical case the numerical methods are not supposed to produce a solution on the whole interval in question, but rather give the solution on a prescribed set of nodes on the given interval. We assume that the nodes are arranged equispaced inside the interval $[0, X]$ and on its borders with a given step-size h. Additionally the nodes are assumed to be numbered increasingly $x_0, x_1, ..., x_N$, where $N = X/h$, $x_0 = 0$ and $x_N = X$. Furthermore we denote by y_m the approximation of $y(x_m)$ and equally $f_m = f(x_m, y_m)$ as the discretized right-hand side of the differential equation in question. For this setting we will develop the fractional counterpart of the well known classical backward difference method.

3.2.1 A first order fractional backward difference method based on the Grünwald-Letnikov derivative

Let us consider the fractional differential equation as follows

$$^{GL}D^\alpha y(x) = f(x, y(x)), \quad y(0) = 0, \quad 0 < \alpha < 1, \tag{3.31}$$

where the Grünwald-Letnikov differential operator, i.e. $^{GL}D^\alpha$, is used. Since $y(0) = 0$ is a homogenous initial condition and by Corollary 2.1.21, the problem (3.31) is equivalent to problem (3.30) for the given case $0 < \alpha < 1$. For the numerical algorithm, we only use a finite sum, s.t $N \in \mathbb{N}$, in Defintion 2.1.19. Then we get the *finite* Grünwald-Letnikov operator

$$^{GL}_F D^\alpha y(x_m) = \frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha}{k} y(x_m - kh), \quad m = 0, 1, ..., N,$$

which thus gives us a discretized version of the operator $^{GL}D^\alpha$. Using the defined mesh points $x_0, ..., x_N$ we therefore get the discretized problem

$$\frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha}{k} y(x_m - kh) = f(x_m, y(x_m)), \quad m = 0, 1, ..., N.$$

If we set $\omega_k = (-1)^k \binom{\alpha}{k}$ we can solve this set of equations one by one at each mesh point x_m by

$$y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^m \omega_k y(x_m - kh), \quad m = 1, ..., N. \tag{3.32}$$

This formula computes the numerical solution of the fractional order differential equation (3.31). We seek the solution at each step, namely y_m, occurs on both sides of equation (3.32). But in each step the mth equation contains y_m as the only unknown quantity, because we have computed $y_1, y_2, ..., y_{m-1}$ in the previous calculations and the solution $y_0 = 0$ is determined by the initial condition in (3.31). Therefore we can solve formula (3.32) for all $m = 1, ..., N$ in a step by step manner. In general, the obtained equations will still be nonlinear so we will have to use a (one-dimensional) fixed point method to solve each of them individually.

Thus formula (3.32) gives us a first order numerical method to solve equation of the type (3.31) as well as equation of type (3.30) given that $0 < \alpha < 1$ and the initial condition is homogenous. For the coefficients ω_k can be computed in a recursive scheme (with $\omega_0 = 1$) by

$$\begin{aligned}
\omega_k &= (-1)^k \binom{\alpha}{k} = (-1)^k \frac{\Gamma(\alpha + 1)}{\Gamma(k+1)\Gamma(\alpha - k + 1)} \\
&= -(-1)^{k-1} \frac{\Gamma(\alpha + 1)(\alpha - k + 1)}{k\Gamma(k)\Gamma(\alpha - k)} = \left(\frac{k - (\alpha + 1)}{k} \right) \omega_{k-1},
\end{aligned}$$

then we have

$$\omega_k = \left(1 - \frac{\alpha+1}{k}\right)\omega_{k-1}, \ \forall \ k \in \mathbb{N}. \tag{3.33}$$

Another way to compute the coefficients ω_k is by their generating function

$$\omega(\zeta) = (1-\zeta)^\alpha, \tag{3.34}$$

i.e. the first k Taylor coefficients of (3.34) are the first k weights ω_k. We note that the generating function (3.34) is the generating function of the first order backward difference method (see formula (1.9)) for the case $\alpha = 1$. Thus by Theorem 3.1.14 we know that formula (3.32) is convergent of order 1 in the sense of Definition 3.1.2. This fact seems to be widely misunderstood to imply that the error of formula (3.32) should behave as $O(h)$ for a finite h. This interpretation is of course not entirely correct as we see by investigating in the last remarks of Section 3.1, which states that we need one additional starting weight at each step given by

$$w_m = \frac{m^{-\alpha}}{\Gamma(1-\alpha)} - (-1)^m \frac{\Gamma(\alpha)}{\Gamma(\alpha-m)\Gamma(m+1)}.$$

Thus we get

$$w_m = \frac{m^{-\alpha}}{\Gamma(m-\alpha)} - \sum_{j=0}^{m} \omega_j, \tag{3.35}$$

then the modified formula becomes

$$y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^{m} \omega_k y(x_m - kh) - \left(\frac{m^{-\alpha}}{\Gamma(m-\alpha)} - \sum_{j=0}^{m} \omega_j\right) y_0, \quad m = 1, ..., N, \tag{3.36}$$

whose error behaves like $O(h)$. Obviously formulas (3.32) and (3.36) are identical if homogenous initial conditions are given, which might be the reason behind the mentioned misunderstanding.

Now we generalize problem (3.31) to the case, where $\alpha > 0$ and the corresponding initial conditions are not necessary homogenous. Thus from Corollary 2.1.21 and Theorem 2.1.15 with Definition 1.1.9 we can rewrite

$$\begin{aligned} {}^C D^\alpha y(x) &= {}^{GL} D^\alpha (y(x) - T_{n-1}[y;0](x)) \\ &= {}^{GL} D^\alpha y(x) - D^\alpha T_{n-1}[y;0](x) \end{aligned}$$

where $y(x)$ is assumed to be n times continuously differentiable. Applied to our problem (3.30) the Taylor polynomial $T_{n-1}[y;0](x)$ is completely defined by the initial conditions and thus we can rewrite formula (3.36) in the case of $\alpha > 0$ to

$$y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^{m} \omega_k y(x_m - kh) - \left(\frac{m^{-\alpha}}{\Gamma(m-\alpha)} - \sum_{j=0}^{m} \omega_j\right) y_0 + h^\alpha \sum_{k=0}^{n-1} \frac{y_0^{(k)} x_m^{k-\alpha}}{\Gamma(k+1-\alpha)}, \quad m = 1, ..., N, \tag{3.37}$$

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All the arguments we stated on formulas (3.32) and (3.36) still apply. We thus have obtained a numerical method of first order to solve fractional differential equations of Caputo type with linear or nonlinear right-hand side and homogenous or inhomogeneous initial conditions for all $\alpha > 0$.

3.2.2 Lubich's fractional backward difference methods

We are now going to construct higher-order backward difference methods for fractional order differential equations based on their classical counterparts. We prepared the analytical background in Section 3.1, where we considered fractional linear multi-step methods, to which fractional backward difference methods form a subset. Hairer, Lubich and Schlichte in [81] are studied the numerical solution for a special type of Volterra integral equations. Lubich's results apply for many important kinds of fractional linear multistep method (see e.g. [112, 113, 114, 117]), but here we will especially be interested in the generalization of classical backward difference methods to the fractional case, which we will denote as *Lubich's fractional backward difference methods*. At the beginning we will repeat some important analytical results to describe the method: Given an Abel-Volterra integral equation of the form (3.25) with a bounded kernel $K(x, t, y(t))$ and a given forcing function $g(x)$, then the FLMM defined by

$$y_m = g(x_m) + h^\alpha \sum_{j=0}^{m} \omega_{m-j} K(x_m, x_j, y(x_j)) + h^\alpha \sum_{j=0}^{s} w_{m,j} K(x_m, x_j, y(x_j)), \tag{3.38}$$

gives an approximation to the true solution $y(x_m)$, whose error satisfies

$$\max_{0 \le m \le N} |y_m - y(x_m)| = O(h^{p-\epsilon}), \tag{3.39}$$

with a small $\epsilon \ge 0$. In (3.38) the convolution weights ω_m are given by the generating function

$$\omega^\alpha(\zeta) = \left(\frac{\sigma(1/\zeta)}{\rho(1/\zeta)} \right)^\alpha \tag{3.40}$$

where (ρ, σ) are the characteristic polynomials of a classical LMM and the starting weights $w_{m,j}$ are given by the linear equation system

$$\sum_{j=0}^{s} w_{m,j} j^\gamma = \frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma+\alpha)} m^{\alpha+\gamma} - \sum_{j=1}^{m} \omega_{m-j} j^\gamma, \ \gamma \in \mathcal{A} \tag{3.41}$$

with

$$\mathcal{A} = \{\gamma = k + j\alpha; \ k, j \in \mathbb{N}_0, \ \gamma \le p - 1\}, \ card\mathcal{A} = s + 1. \tag{3.42}$$

Furthermore in Lemma 2.2.3 we have seen how the fractional differential equation (3.30) can be transferred to the following Abel-Volterra integral equation

$$y(x) = T_{n-1}[y; 0](x_m) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt \tag{3.43}$$

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where the forcing function $T_{n-1}[y;0](x_m)$ is completely defined by the initial conditions of (3.30) and the kernel $K(t,x,y(x)) = f(x,y(x))$ is given by the right-hand side of (3.30).

Finally, in Example 1.1.27 we have seen that the classical backward difference method of order p possesses the generating function

$$\omega(\zeta) = \sum_{k=0}^{p} \omega_k \zeta^k = \sum_{k=1}^{p} \frac{1}{k}(1-\zeta)^k. \tag{3.44}$$

With these results we can describe Lubich's fractional backward difference method by:

Theorem 3.2.1. *Let $\alpha > 0$ and $n = \lceil \alpha \rceil$. Lubich's fractional backward difference method of order $p \in \{1,...,6\}$ for a fractional differential equation of Caputo type (3.30) rewritten as Abel-Volterra integral equation (3.43) is given by*

$$y_m = T_{n-1}[y;0](x_m) + h^\alpha \sum_{j=0}^{m} \omega_{m-j} f(x_j, y(x_j)) + h^\alpha \sum_{j=0}^{s} w_{m,j} f(x_j, y(x_j)) \tag{3.45}$$

for $m = 1,...,N$, where the convolution weights ω_m are given by the generating function

$$\omega^\alpha(\zeta) = \left(\sum_{k=1}^{p} \frac{1}{k}(1-\zeta)^k \right)^{-\alpha}$$

and the starting weights $w_{m,j}$ are given by the solution of the linear equation system (3.41). Equation (3.45) gives an approximation of order $O(h^{p-\epsilon})$ with a small $\epsilon \geq 0$ for all fixed mesh points x_m.

Even though we could use Theorem 3.2.1 directly as numerical method to solve fractional differential equations, it is more reasonable to use the following method

Theorem 3.2.2. *Let $\alpha > 0$ and $n = \lceil \alpha \rceil$. Lubich's fractional backward difference method of order $p \in \{1,...,6\}$ for a fractional differential equation of Caputo type (3.30) is given by*

$$y_m = h^\alpha f(x_m, y_m) - \sum_{j=0}^{m-1} \omega_{m-j} y(x_j) - \sum_{j=0}^{s} w_{m,j} y(x_j) + h^\alpha \, {}^C D^\alpha T_{n-1}[y;0](x_m) \tag{3.46}$$

for $m = 1,...,N$, where the convolution weights ω_m are given by the generating function

$$\omega^\alpha(\zeta) = \left(\sum_{k=1}^{p} \frac{1}{k}(1-\zeta)^k \right)^{\alpha} \tag{3.47}$$

and the starting weights $w_{m,j}$ are given by the solution of the linear equation system

$$\sum_{j=0}^{s} w_{m,j} j^\gamma = \frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma-\alpha)} m^{\gamma-\alpha} - \sum_{j=1}^{m} \omega_{m-j} j^\gamma, \ \gamma \in \mathcal{A} \tag{3.48}$$

with $\mathcal{A}$ as defined in (3.42). The weights $w_{m,j}$ are of order $O(m^{-\alpha-1})$ and the error satisfies $O(h^{p-\epsilon})$ with a small $\epsilon \geq 0$ for all fixed mesh points x_m.

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Remark 3.2.3. **(a)** The restriction of order $p \in \{1, ..., 6\}$ is based on the fact that the classical backward difference methods are stable only up to order $p = 6$ (see e.g. [83]), which is a necessary condition of Theorem 3.1.14 for the stability of the fractional backward difference method.

(b) The 'small value ϵ' in Theorem 3.2.1 and Theorem 3.2.2 is given by the following equation,

$$\epsilon = p - \alpha - \min\{\gamma = k + j\alpha, \ k, j \in \mathbb{N}_0, \ \gamma > p - 1\},$$

and thus in particular is zero for $\alpha = q/(q+1)$ with $q \in \mathbb{N}$.

(c) Obviously, we can summarize the stated results as follow:

- A (non)linear fractional order differential equation of Caputo type with $\alpha > 0$ can be solved by formula (3.46), where in the first $s+1$ steps a (non)linear equations system and in each step $m = s + 1, ..., N$ a (non)linear equation has to be solved.

- The error at any fixed mesh point is given by $O(h^{p-\epsilon})$ with small $\epsilon \geq 0$ where the choice of p and the order α of the fractional differential equation determine the parameter s, given by $card\mathcal{A} - 1$ with $\mathcal{A}$ defined in (3.42), as well as the weights ω_m and $w_{m,j}$ given by the generating function (3.47) and the linear equation system (3.48) respectively.

- In case of homogenous initial conditions, formula (3.46) without the term $h^\alpha \ ^C D^\alpha T_{n-1}$ $[y; 0](x_m)$ describes a fractional backward difference methods of order p for fractional differential equations of Caputo type.

With Theorem 3.2.2 we have established a generalization of the classical backward difference methods to the fractional case. This means we focused our attention on the analytical results, i.e. the fractional differential equation (3.30) has a numerical solution, given by formula (3.46), on the interval $[0, X]$. In this solution the only unknowns are the convolution weights ω_m, which are given by their generating function (3.47), the starting weights $w_{m,j}$, which are given by the solution of the linear equation system (i.e. (3.48), where the set $\mathcal{A}$ is dependent of α and p and defined by (3.42)). Another important point is the implementation of the higher-order backward difference method based on Lubich's work described in this subsection. Thus, for an implemention of these results, we refer for more details to [49, 66].

In the next section we discuss another numerical method, which is based on fractional linear multistep methods.

3.3 Fractional Adams-Moulton (FAM) methods

In this section we consider the problem of numerically solving the following FODE (i.e. Cauchy problem)

$$^C D^\alpha y(x) = f(x, y(x)), \ y(0) = y_0 \tag{3.49}$$

by means of a generalization of k-step Adams-Moulton multistep methods. Where $f : [0, X] \times \mathbb{R} \to \mathbb{R}$ is a sufficiently smooth function and $0 < \alpha < 1$. From the viewpoint of FLMMs (see Theorem 3.2.1), we can write

$$y_n = y_0 + h^\alpha \sum_{j=0}^{s} w_{n,j} f(x_j, y_j) + h^\alpha \sum_{j=0}^{n} \omega_{n-j} f(x_j, y_j). \tag{3.50}$$

In [64], FLMMs can be conveniently rewritten in the form of classic linear multistep methods by the following way

$$\sum_{j=0}^{n} \beta_j (y_{n-j} - y_0) + \sum_{j=0}^{s} a_{n,j}(y_j - y_0) = h^\alpha \sum_{j=0}^{n} \gamma_j f(x_{n-j}, y_{n-j}), \tag{3.51}$$

where weights β_j, γ_j and ω_j are coefficients in the expansion of $\beta(\zeta)$, $\gamma(\zeta)$ and $\omega(\zeta)$, respectively, and $\omega(\zeta) = \gamma(\zeta)/\beta(\zeta)$. Moreover starting weights $a_{n,j}$ are linear function of $w_{n,j}$, ω_j and β_j.

Now, we will come back to describe the FAM methods. First, in the numerical treatment of ODEs, a k-step scheme of Adams type is usually written in the form

$$y_n - y_{n-1} = h \sum_{j=0}^{k} \bar{\gamma}_j \nabla^j f_n,$$

where $\bar{\gamma}_j$ are the real coefficients, h is the step-size $h = x_n - x_{n-1}$ and $\nabla^j f_n = \nabla^j f(x_n, y_n)$ denote backward differences of f. By expressing differences $\nabla^j f_n$ in terms of values f_{n-j}, according to $\nabla^j f_n = \sum_{i=0}^{j} (-1)^i \binom{j}{i} f_{n-j}$, k-step Adams methods can also be written in the form

$$y_n - y_{n-1} = h \sum_{j=0}^{k} \bar{\gamma}_j^{(k)} f_{n-j}$$

where

$$\bar{\gamma}_j^{(k)} = (-1)^j \sum_{l=j}^{k} \binom{l}{j} \bar{\gamma}_l, \ \ j = 0, 1, ..., k. \tag{3.52}$$

Coefficients $\bar{\gamma}_j$ can be determined by evaluating the coefficients of the first powers of a variable ζ in the asymptotic expansion of a generating function $G(\zeta)$ (e.g., see [95]).

We can extend this method to FDEs, by considering a suitable expansion of the α-power of the generating function $G(\zeta) = (-\zeta/\ln(1-\zeta))$ (i.e. the generating function of Adams-Moulton

for ODEs). It was Lubich [113] who first used form of convolution quadrature (3.50) to investigate this approach and, in [64] have been addressed by the formula (3.51). In general, the α-power of the generating function $G(t) = (-t/\ln(1-t))$ can be written as

$$(G(t))^\alpha = \left(-\frac{\ln(1-t)}{t} \right)^{-\alpha} = \left(1 + \sum_{k=2}^{\infty} \frac{t^{k-1}}{k} \right)^{-\alpha}. \tag{3.53}$$

Thus, we can state the J.C.P. Miller formula for the power of a power series by the following theorem (Theorem 1.6c [84]).

Theorem 3.3.1. *Let $P(t) = 1 + \sum_{k=1}^{\infty} a_k t^k$ be a formal unitary series. Then for any $r \in \mathbb{C}$,*

$$(P(t))^r = \sum_{n=0}^{\infty} V_n^{(r)} t^n,$$

where coefficients $V_n^{(r)}$ can be recursively evaluated as

$$V_0^{(r)} = 1, \quad V_n^{(r)} = \sum_{j=1}^{n} \left(\frac{(r+1)j}{n} - 1 \right) a_j V_{n-j}^{(r)}.$$

By applying Theorem 3.3.1, we have now

$$(G(t))^\alpha = \sum_{n=0}^{\infty} \gamma_n t^n,$$

where

$$\gamma_0 = 1, \quad \gamma_n = \sum_{j=1}^{n} \left(\frac{(1-\alpha)j - n}{n(j+1)} \right) \gamma_{n-j}, \ n = 1, 2, ..., \tag{3.54}$$

and the first six coefficients are given by

$$
\begin{aligned}
\gamma_0 &= 1, \\
\gamma_1 &= -\frac{\alpha}{2}, \\
\gamma_2 &= \frac{1}{8}\alpha^2 - \frac{5}{24}\alpha, \\
\gamma_3 &= -\frac{1}{48}\alpha^3 + \frac{5}{48}\alpha^2 - \frac{1}{8}\alpha, \\
\gamma_4 &= \frac{1}{384}\alpha^4 - \frac{5}{192}\alpha^3 + \frac{97}{1152}\alpha^2 - \frac{251}{2880}\alpha, \\
\gamma_5 &= -\frac{1}{3840}\alpha^5 + \frac{5}{1152}\alpha^4 - \frac{61}{2304}\alpha^3 + \frac{401}{5760}\alpha^2 - \frac{19}{288}\alpha.
\end{aligned}
\tag{3.55}
$$

Now, we can define a k-step fractional Adams-Moulton method as a FLMM obtained by means of the generating function

$$\omega^\alpha(\zeta) = \frac{\gamma_0 + \gamma_1(1 - \zeta) + \dots + \gamma_k(1 - \zeta)^k}{(1 - \zeta)^\alpha}. \tag{3.56}$$

In order to write (3.56) in the form of formula (3.51), we expand $(1 - \zeta)^\alpha = \sum_{j=0}^{\infty} \omega_j \zeta^j$, where coefficients ω_j can be recursively evaluated as

$$\omega_0 = 1, \quad \omega_j = \left(1 - \frac{\alpha + 1}{j}\right)\omega_{j-1}, \ j = 1, 2, \dots,$$

and we rewrite $\sum_{j=0}^{k} \gamma_j(1 - \zeta)^j$ in powers of ζ instead of $(1 - \zeta)$ by using (3.52). By means of formula (3.51), a k-step FAM method can therefore be written as

$$\sum_{j=0}^{n} \omega_j(y_{n-j} - y_0) + \sum_{j=0}^{s} a_{n,j}(y_j - y_0) = h^\alpha \sum_{j=0}^{k} \gamma_j^{(k)} f(x_{n-j}, y_{n-j}), \tag{3.57}$$

where coefficients $\gamma_j^{(k)}$ are given in the paper of Galeone and Garrappa by (Tables 1-2 [64]).

Remark 3.3.2. **(a)** The case $k = 0$ formula (3.57) corresponds to the first order backward differential fromula (3.32) (see Subsection 3.2.1). Also, if $\alpha \to 1$ coefficients of Adams-Moulton methods for ODEs are obtained.

(b) FAM method can be obtained by means of multistep method (3.50) where the coefficients γ_n in the α-power of the generating function ω (see Lemma 3.1.7) can be calculated by fromula (3.54) and the first terms are given by (3.55).

Chapter 4

A predictor-corrector approach for the numerical solution of FODEs

In order to give the reader a tool that can be applied to a very wide class of equations, here we present an Adams-type predictor- corrector method [40, 41] that is well understood and that has proven to be efficient in many practical applications (see e.g. [42, 43, 62, 164, 165]). Before starting the investigations, we need to give a note of caution. As seen in Chapter 2 that in general there exists more than one way to transfer results of classical calculus to the fractional case, which lead e.g. to the different definitions of fractional derivatives. We have like this behaviour, for analyzing numerical methods of the FODEs. Therefore, we should give the following remark.

Remark 4.0.1. As we have seen in Chapter 3 that it is common to construct methods for fractional differential equations by taking methods for classical (typically first-order) equations and then to generalize the concepts in an appropriate way. The obvious way to denote these methods is then to give them the same name as the underlying classical algorithm, possibly extended by the adjective "fractional". However, many classical numerical schemes can be extended in more than one way, which may lead to the problem that, in two different items of literature, two different algorithms are denoted by the same name. For example, the fractional Adams-Moulton method (see Section 3.3) of Galeone and Garrappa [64] do not coincide with the methods of the same name that we will consider below.

4.1 The predictor-corrector algorithm

We now introduce a numerical method to solve the fractional differential equation of Caputo type (3.30) based on the fractional formulation of the classical Adams-Bashforth-Moulton method. In particular we will use the formulation of the problem in Abel-Volterra integral form

$$y(x) = \sum_{k=0}^{n-1} \frac{x^k}{k!} y_0^{(k)} + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt. \tag{4.1}$$

This method has been introduced and briefly discussed in [42] and some more information is given in [43]. A number of additional results for a specific initial value problem are contained in [44], a detailed mathematical analysis is provided in [45], and additional practical remarks can be found in [40]. Numerical experiments and comparisons with other methods are reported in [46, 62, 164, 165].

In Example 1.1.26 we have briefly explained the Adams-type formulas for the classical case. We will now develop similar formulas for the fractional case. We assume that a unique solution of (4.1) exists on some interval $[0, X]$ and that we are interested in a numerical solution on the uniform grid $\{x_j = jh : j = 0, 1, ..., N\}$ with some integer N and step-size $h = X/N$. Assuming that we have already calculated the approximations $y_j \approx y(x_j)$, $j = 1, 2, ..., k$, the basic idea is to obtain the solution y_{k+1} by replacing the equation (4.1) with a discrete formula. What we do is simply use the product trapezoidal quadrature formula to replace the integral in (4.1), i.e. we use the nodes x_j, $j = 0, 1, ..., k+1$ and interpret the function $(x_{k+1} - .)^{\alpha-1}$ as a weight function for the integral. In other words, we apply the approximation

$$\int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} g(z) dz \approx \int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} \tilde{g}_{k+1}(z) dz, \tag{4.2}$$

where $\tilde{g}_{k+1}$ is the piecewise linear interpolant for g with nodes and knots chosen at the x_j, $j = 0, 1, 2, ..., k+1$. It is clear by construction that the required weighted trapezoidal quadrature formula can be represented as a weighted sum of function values of the integrand g, taken at the points x_j. Specifically, we find that we can write the integral on the right-hand side of (4.2) as

$$\int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} \tilde{g}_{k+1}(z) dz = \sum_{j=0}^{k+1} a_{j,k+1} g(x_j) \tag{4.3}$$

where

$$a_{j,k+1} = \int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} \phi_{j,k+1}(z) dz \tag{4.4}$$

and

$$\phi_{j,k+1}(z) = \begin{cases} (z - x_{j-1})/(x_j - x_{j-1}) & \text{if} \quad x_{j-1} < z \le x_j, \\ (x_{j+1} - z)/(x_{j+1} - x_j) & \text{if} \quad x_j < z < x_{j+1}, \\ 0 & \text{else.} \end{cases} \tag{4.5}$$

This is clear because the functions $\phi_{j,k+1}$ satisfy

$$\phi_{j,k+1}(x_\mu) = \begin{cases} 0 & \text{if} \quad j \ne \mu, \\ 1 & \text{if} \quad j = \mu, \end{cases}$$

and that they are continuous and piecewise linear with breakpoints at the nodes x_μ, so that they must be integrated exactly by our formula.

An easy explicit calculation yields that, for an arbitrary choice of the x_j, (4.4) and (4.5) produce

$$a_{0,k+1} = \frac{(x_{k+1} - x_1)^{\alpha+1} + x_{k+1}^{\alpha}[\alpha x_1 + x_1 - x_{k+1}]}{x_1 \alpha(\alpha+1)},$$ (4.6)

$$a_{j,k+1} = \frac{(x_{k+1} - x_{j-1})^{\alpha+1} + (x_{k+1} - x_j)^{\alpha}[\alpha(x_{j-1} - x_j) + x_{j-1} - x_{k+1}]}{(x_j - x_{j-1})\alpha(\alpha+1)}$$

$$+ \frac{(x_{k+1} - x_{j+1})^{\alpha+1} - (x_{k+1} - x_j)^{\alpha}[\alpha(x_j - x_{j+1}) - x_{j+1} + x_{k+1}]}{(x_{j+1} - x_j)\alpha(\alpha+1)},$$ (4.7)

if $1 \le j \le k$, and

$$a_{k+1,k+1} = \frac{(x_{k+1} - x_k)^{\alpha}}{\alpha(\alpha+1)}.$$ (4.8)

In the case of equispaced nodes ($x_j = jh$ with some fixed h), these relations reduce to

$$a_{j,k+1} = \frac{h^{\alpha}}{\alpha(\alpha+1)} \times \begin{cases} (k^{\alpha+1} - (k-\alpha)(k+1)^{\alpha}) & \text{if} \quad j = 0, \\ ((k-j+2)^{\alpha+1} + (k-j)^{\alpha+1} - 2(k-j+1)^{\alpha+1}) & \text{if} \quad 1 \le j \le k, \\ 1 & \text{if} \quad j = k+1. \end{cases}$$ (4.9)

This then gives us our corrector formula (i.e. the fractional variant of the one-step *Adams-Moulton method*), which is

$$y_{k+1} = \sum_{j=0}^{n-1} \frac{x_{k+1}^j}{j!} y_0^{(j)} + \frac{1}{\Gamma(\alpha)} \left(\sum_{j=0}^{k} a_{j,k+1} f(x_j, y_j) + a_{k+1,k+1} f(x_{k+1}, y_{k+1}^P) \right).$$ (4.10)

The remaining problem is the determination of the predictor formula that we require to calculate the value y_{k+1}^P. The idea we use to generalize the one-step Adams-Bashforth method is the same as the one described above for the Adams-Moulton technique: We replace the integral on the right-hand side of equation (4.1) by the product rectangle rule

$$\int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} g(z) dz \approx \sum_{j=0}^{k} b_{j,k+1} g(x_j),$$ (4.11)

where now

$$b_{j,k+1} = \int_{x_j}^{x_{j+1}} (x_{k+1} - z)^{\alpha-1} dz = \frac{(x_{k+1} - x_j)^{\alpha} - (x_{k+1} - x_{j+1})^{\alpha}}{\alpha}.$$ (4.12)

This expression for weights can be derived in a way similar to the method used in the derivation of $a_{j,k+1}$. However, here we are dealing with a piecewise constant approximation and not a piecewise linear one, and hence we have to replace the "hat-shaped" functions ϕ_{kj} by functions being of constant value 1 on $[x_j, x_{j+1}]$ and 0 on the remaining parts of the interval $[0, x_{k+1}]$. Again, in the equispaced case, we have the simpler expression

$$b_{j,k+1} = \frac{h^\alpha}{\alpha}((k+1-j)^\alpha - (k-j)^\alpha). \tag{4.13}$$

Thus, the predictor y_{k+1}^P is determined by the fractional *Adams-Bashforth method* (that is, the fractional Euler method)

$$y_{k+1}^P = \sum_{j=0}^{n-1} \frac{x_{k+1}^j}{j!} y_0^{(j)} + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{k} b_{j,k+1} f(x_j, y_j). \tag{4.14}$$

Our basic algorithm, the fractional Adams-Bashforth-Moulton method, is thus completely described by equations (4.10) and (4.14) with the weights $a_{j,k+1}$ and $b_{j,k+1}$ being defined according to (4.9) and (4.13), respectively. Obviously, we first have to calculate the predictor y_{k+1}^P according to equation (4.14), then we evaluate $f(x_{k+1}, y_{k+1})$, use this to determine the corrector y_{k+1} by means of equation (4.10), and finally evaluate $f(x_{k+1}, y_{k+1})$ which is then used in the next integration step. Therefore, methods of this type are frequently called predictor-corrector or, more precisely, PECE (Predict, Evaluate, Correct, Evaluate) methods.

4.2 Error Analysis

For the error analysis of this algorithm, we restrict our attention to the case of an equispaced grid, i.e. from now on we assume that $x_j = jh = jX/N$ with some $N \in \mathbb{N}$. Essentially we follow the structure of [45] and begin by stating some auxiliary results.

What we do need for our purposes is some information on the errors of the quadrature formulas that we have used in the derivation of the predictor and the corrector, respectively. We first give a statement on the product rectangle rule that we have used for the predictor.

Theorem 4.2.1. (a) *Let $z \in C^1[0, X]$. Then,*

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} z(x) dx - \sum_{j=0}^{k} b_{j,k+1} z(t_j) \right| \leq \frac{1}{\alpha} \|z'\|_\infty \, x_{k+1}^\alpha h.$$

(b) *Let $z(x) = x^p$ for some $p \in (0,1)$. Then,*

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} z(x) dx - \sum_{j=0}^{k} b_{j,k+1} z(t_j) \right| \leq C_{\alpha,p}^{\mathrm{Re}} \, x_{k+1}^{\alpha+p-1} h,$$

where $C_{\alpha,p}^{\mathrm{Re}}$ is a constant that depends only on α and p.

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Proof. By construction of the product rectangle formula, we find in both cases that the quadrature error has the representation

$$\int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} z(x) dx - \sum_{j=0}^{k} b_{j,k+1} z(x_j)$$

$$= \sum_{j=0}^{k} \int_{jh}^{(j+1)h} (x_{k+1} - x)^{\alpha-1} (z(x) - z(x_j)) dx. \qquad (4.15)$$

To prove statement (a), we apply the Mean Value Theorem of differential calculus to the second factor of the integrand on the right-hand side of (4.15) and derive

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} z(x) dx - \sum_{j=0}^{k} b_{j,k+1} z(t_j) \right|$$

$$\leq \|z'\|_\infty \sum_{j=0}^{k} \int_{jh}^{(j+1)h} (x_{k+1} - x)^{\alpha-1} (x - jh) dx$$

$$= \|z'\|_\infty \frac{h^{1+\alpha}}{\alpha} \sum_{j=0}^{k} \left(\frac{1}{1+\alpha} [(k+1-j)^{1+\alpha} - (k-j)^{1+\alpha}] - (k-j)^{\alpha} \right)$$

$$= \|z'\|_\infty \frac{h^{1+\alpha}}{\alpha} \left(\frac{(k+1)^{1+\alpha}}{1+\alpha} - \sum_{j=0}^{k} j^{\alpha} \right)$$

$$= \|z'\|_\infty \frac{h^{1+\alpha}}{\alpha} \left(\int_0^{k+1} x^{\alpha} dx - \sum_{j=0}^{k} j^{\alpha} \right).$$

Here the term in parentheses is simply the remainder of the standard rectangle quadrature formula, applied to the function x^{α}, and taken over the interval $[0, k+1]$. Since the integrand is monotonic, we may apply some standard results from quadrature theory [19, Theorem 97 0912] to find that this term is bounded by the total variation of the integrand, viz. the quantity $(k+1)^{\alpha}$. Thus,

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} z(x) dx - \sum_{j=0}^{k} b_{j,k+1} z(x_j) \right| \leq \|z'\|_\infty \frac{h^{1+\alpha}}{\alpha} (k+1)^{\alpha}.$$

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Similarly, to prove (b), we use the monotonicity of z in (4.15) and derive

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha - 1} z(x) dx - \sum_{j=0}^{k} b_{j,k+1} z(x_j) \right|$$

$$\leq \sum_{j=0}^{k} |z(x_{j+1}) - z(x_j)| \int_{jh}^{(j+1)h} (x_{k+1} - x)^{\alpha - 1} dx$$

$$= \frac{h^{\alpha + p}}{\alpha} \sum_{j=0}^{k} ((j+1)^p - j^p)((k+1-j)^\alpha - (k-j)^\alpha)$$

$$\leq \frac{h^{\alpha + p}}{\alpha} \left((k+1)^\alpha - k^\alpha + (k+1)^p - k^p + p\alpha \sum_{j=1}^{k-1} j^{p-1}(k-j+q)^{\alpha - 1} \right)$$

$$\leq \frac{h^{\alpha + p}}{\alpha} \left(n(k+q)^{\alpha - 1} + pk^{p-1} + p\alpha \sum_{j=1}^{k-1} j^{p-1}(k-j+q)^{\alpha - 1} \right).$$

by additional applications of the Mean Value Theorem. Here $q = 0$ if $\alpha \leq 1$, and $q = 1$ otherwise. In either case a brief asymptotic analysis using the Euler-MacLaurin formula ([173], Theorem 3.7) yields that the term in parentheses is bounded from above by $C_{\alpha,p}^{\mathrm{Re}} (k+1)^{p+\alpha - 1}$ where $C_{\alpha,p}^{\mathrm{Re}}$ is a constant depending on α and p but not on k. □

Next we come to a corresponding result for the product trapezoidal formula that we have used for the corrector. The proof of this theorem is very similar to the proof of Theorem 4.2.1. We therefore state the following theorem without proof.

Theorem 4.2.2. (a) *If* $z \in C^2[0, X]$ *then there is a constant* C_α^{Tr} *depending only on* α *such that*

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha - 1} z(x) dx - \sum_{j=0}^{k+1} a_{j,k+1} z(x_j) \right| \leq C_\alpha^{\mathrm{Tr}} \|z''\|_\infty x_{k+1}^\alpha h^2.$$

(b) *Let* $z \in C^1[0, X]$ *and assume that* z' *fulfils a Lipschitz condition of order* μ *for some* $\mu \in (0, 1)$. *Then, there exist positive constants* $B_{\alpha,\mu}^{Tr}$ *(depending only on* α *and* μ*) and* $M(z, \mu)$ *(depending only on* z *and* μ *) such that*

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha - 1} z(x) dx - \sum_{j=0}^{k+1} a_{j,k+1} z(t_j) \right| \leq B_{\alpha,\mu}^{\mathrm{Tr}} M(z, \mu) x_{k+1}^\alpha h^{1+\mu}.$$

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(c) *Let $z(x) = x^p$ for some $p \in (0,2)$ and $\rho := \min(2, p+1)$. Then,*

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} z(x) dx - \sum_{j=0}^{k+1} a_{j,k+1} z(x_j) \right| \leq C_{\alpha,p}^{\mathrm{Tr}} \ x_{k+1}^{\alpha+p-\rho} \ h^\rho,$$

where $C_{\alpha,p}^{\mathrm{Tr}}$ is a constant that depends only on α and p.

It may happen that $\alpha < 1$, $p < 1$ in part (b) of Theorem 4.2.1 and in part (c) of Theorem 4.2.2. For a details of this remark we refer to ([45], Remark 2.1).

We now present the main results of this section, namely, the theorems concerning the error of our Adams scheme. It is useful to distinguish a number of cases. Specifically, we shall see that the precise behaviour of the error differs depending on whether $\alpha < 1$ or $\alpha > 1$. Moreover, the smoothness properties of the given function f and the unknown solution y play an important role. In view of the results of Subsection 2.2.3, we find that smoothness of one of these functions will imply non-smoothness of the other unless some special conditions are fulfilled. Therefore we shall also investigate the error under those two different smoothness assumptions.

Based on the error estimates above we shall first present a general convergence result for the Adams-Bashforth-Moulton method. In the theorems below we shall specialize this result to particularly important special cases.

Lemma 4.2.3. *Assume that the solution y of the initial value problem is such that*

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} \ {}^C D^\alpha y(x) dx - \sum_{j=0}^{k} b_{j,k+1} \ {}^C D^\alpha y(x_j) \right| \leq C_1 \ x_{k+1}^{\gamma_1} h^{\delta_1}$$

and

$$\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} \ {}^C D^\alpha y(x) dx - \sum_{j=0}^{k+1} a_{j,k+1} \ {}^C D^\alpha y(x_j) \right| \leq C_2 \ x_{k+1}^{\gamma_2} h^{\delta_2}$$

with some $\gamma_1, \gamma_2 \geq 0$ and $\delta_1, \delta_2 > 0$. Then, for some suitalbly chosen $X > 0$, we have

$$\max_{0 \leq j \leq N} |y(x_j) - y_j| = O(h^q)$$

where $q = \min\{\delta_1 + \alpha, \delta_2\}$ and $N = \lfloor X/h \rfloor$.

Proof. We will show that, for sufficiently small h,

$$|y(x_j) - y_j| \leq C h^q \tag{4.16}$$

for all $j \in \{0, 1, ..., N\}$, where C is a suitable constant. The proof will be based on mathematical induction. In view of the given initial condition, the induction basis ($j = 0$) is presupposed. Now assume that (4.16) is true for $j = 0, 1, ..., k$ for some $k \leq N - 1$. We must then prove that the

inequality also holds for $j = k + 1$. To do this, we first look at the error of the predictor y_{k+1}^P. By construction of the predictor we find that

$$
\begin{aligned}
|y(x_{k+1}) - y_{k+1}^P| \quad &= \quad \frac{1}{\Gamma(\alpha)}\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} f(x, y(x))dx - \sum_{j=0}^k b_{j,k+1} f(x_j, y_j) \right| \\
&\leq \quad \frac{1}{\Gamma(\alpha)}\left| \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1}\,{}^C D^\alpha y(x)dx - \sum_{j=0}^k b_{j,k+1}\,{}^C D^\alpha y(x_j) \right| \\
&\quad + \quad \frac{1}{\Gamma(\alpha)} \sum_{j=0}^k b_{j,k+1} |f(x_j, y(x_j)) - f(x_j, y_j)| \\
&\leq \quad \frac{C_1 x_{k+1}^{\gamma_1}}{\Gamma(\alpha)} h^{\delta_1} + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^k b_{j,k+1} LCh^q \\
&\leq \quad \frac{C_1 X^{\gamma_1}}{\Gamma(\alpha)} h^{\delta_1} + \frac{CLX^\alpha}{\Gamma(\alpha+1)} h^q. \qquad\qquad\qquad (4.17)
\end{aligned}
$$

Here we have used the Lipschitz property of f, the assumption on the error of the rectangle formula, and the facts that, by construction of the quadrature formula underlying the predictor, $b_{j,k+1} > 0$ for all j and k and

$$
\sum_{j=0}^k b_{j,k+1} = \int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} dx = \frac{1}{\alpha} x_{k+1}^\alpha \leq \frac{1}{\alpha} X^\alpha.
$$

On the basis of the bound (4.17) for the predictor error we begin the analysis of the corrector error. We recall the relation (4.9) which we shall use, in particular, for $j = k+1$ and find, arguing in a similar way to above, that

$$
\begin{aligned}
|y(x_{k+1}) - y_{k+1}| = \frac{1}{\Gamma(\alpha)}\Bigg| &\int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1} f(x, y(x))dx \\
&- \sum_{j=0}^k a_{j,k+1} f(x_j, y_j) - a_{k+1,k+1} f(x_{k+1}, y_{k+1}^P) \Bigg| \\
\leq \frac{1}{\Gamma(\alpha)}\Bigg| &\int_0^{x_{k+1}} (x_{k+1} - x)^{\alpha-1}\,{}^C D^\alpha y(x)dx - \sum_{j=0}^{k+1} a_{j,k+1}\,{}^C D^\alpha y(x_j) \Bigg| \\
&+ \frac{1}{\Gamma(\alpha)} \sum_{j=0}^k a_{j,k+1} |f(x_j, y(x_j)) - f(x_j, y_j)| \\
&+ \frac{1}{\Gamma(\alpha)} a_{k+1,k+1} |f(x_{k+1}, y(x_{k+1})) - f(x_{x+1}, y_{k+1}^P)|.
\end{aligned}
$$

Then, we have

$$|y(x_{k+1}) - y_{k+1}| \le \frac{C_2 x_{k+1}^{\gamma_2}}{\Gamma(\alpha)} h^{\delta_2} + \frac{CL}{\Gamma(\alpha)} h^q \sum_{j=0}^{k} a_{j,k+1} + a_{k+1,k+1} \frac{L}{\Gamma(\alpha)} \left(\frac{C_1 X^{\gamma_1}}{\Gamma(\alpha)} h^{\delta_1} + \frac{CLX^{\alpha}}{\Gamma(\alpha+1)} h^q \right)$$

$$\le \left(\frac{C_2 X^{\delta_2}}{\Gamma(\alpha)} + \frac{CLX^{\alpha}}{\Gamma(\alpha+1)} + \frac{C_1 LX^{\delta_1}}{\Gamma(\alpha)\Gamma(\alpha+2)} + \frac{CL^2 X^{\alpha}}{\Gamma(\alpha+1)\Gamma(\alpha+2)} h^{\alpha} \right) h^q$$

in view of the nonnegativity of γ_1 and γ_2 and the relations $\delta_2 \le q$ and $\delta_1 + n \le q$. By choosing X sufficiently small, we can make sure that the second summand in the parentheses is bounded by $C/2$. Having fixed this value for X, we can then make the sum of the remaining expressions in the parentheses smaller than $C/2$ too (for sufficiently small h) simply by choosing C sufficiently large. It is then obvious that the entire upper bound does not exceed Ch^q. □

Now, we state the most significant results on the error analysis of the described method, performed in [45]. The first result is based on smoothness assumptions on $^C D^\alpha y$ and given by

Theorem 4.2.4. *Let $\alpha > 0$ and assume $^C D^\alpha y \in C^2[0, X]$ for some suitable X. Then,*

$$\max_{0 \le j \le N} |y(x_j) - y_j| = \begin{cases} O(h^2) & \text{if} \quad \alpha \ge 1, \\ O(h^{1+\alpha}) & \text{if} \quad \alpha < 1. \end{cases} \tag{4.18}$$

Proof. In view of Theorem 4.2.1 and 4.2.2, we may apply Lemma 4.2.3 with $\gamma_1 = \gamma_2 = \alpha > 0$, $\delta_1 = 1$ and $\delta_2 = 2$. Thus, defining

$$q = \min\{1 + \alpha, 2\} = \begin{cases} 2 & \text{if} \quad \alpha \ge 1, \\ 1 + \alpha & \text{if} \quad \alpha < 1, \end{cases}$$

we note that an $O(h^q)$ error bound. □

Remark 4.2.5. The order of convergence depends on α, and it is a non-decreasing function of α. This is due to the discretization of the integral operator in (4.1) which behaves more smoothly (and hence can be approximated with a higher accuracy) as α increases. In contrast, so-called *direct methods* like the backward differentiation method (i.e. Section 3.2), such methods directly discretize the differential operator in the given initial value problem (3.30). The smoothness properties of such operators deteriorate as α increases, and so we note that the convergence order of the method from [47] is a non-increasing function of α; in particular no convergence is achieved there for $\alpha \ge 2$. It is a distinctive advantage of the Adams scheme presented in this section that it converges for all $\alpha > 0$.

We have seen in Subsection 2.2.3 that smoothness of $y(x)$ usually implies non-smoothness of $^C D^\alpha y$. Thus we state as second result on the error behaviour the convergence of the described method with respect to the smoothness of y itself.

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Theorem 4.2.6. *Let $0 < \alpha < 1$ and assume that $y \in C^2[0, X]$ for some suitable X. Then, for $1 \leq j \leq N$ we have*

$$|y(x_j) - y_j| \leq C x_j^{\alpha - 1} \times \begin{cases} h^{1+\alpha} & if \quad 0 < \alpha < 1/2, \\ h^{2-\alpha} & if \quad 1/2 \leq \alpha < 1, \end{cases} \qquad (4.19)$$

where C is a constant independent of j and h.

Proof. A proof of this theorem can be found e.g. in ([45], Theorem 3.4). $\qquad\square$

Thus for all choices of $\alpha > 0$ the described method gives a convergence order of at least one if either y or $^{C}D^{\alpha}y$ is at least two times continuous differentiable on $[0, X]$.

An objection against the use of PECE method may be the very slow rate of convergence if α is close to 0. Thus, the next idea is to find a better approximation for the exact solution of the initial value problem (3.30). There are two main ways to achieve this goal. The first one, we may replace the plain PECE structure by a $P(EC)^M E$ method, i.e. by introducing additional corrector iterations.

Remark 4.2.7. **(a)** An interesting observation here is that by choosing a larger number of corrector iterations M, we essentially leave the computational complexity unchanged: A corrector iteration is of the form (cf. (4.10))

$$y_{j+1}^{[l]} = \sum_{r=0}^{n-1} \frac{x_{j+1}^r}{r!} y_0^{(r)} + \frac{h^\alpha}{\Gamma(\alpha+2)} \left(f(x_{j+1}, y_{j+1}^{[l-1]}) + \sum_{r=0}^{j} a_{r,j+1} f(x_r, y_r) \right), \quad (l = 1, ..., M)$$

Here $y_{j+1}^{[l]}$ denotes the approximation after l corrector steps, $y_{j+1}^{[0]} = y_{j+1}^P$ is the predictor, and $y_{j+1} := y_{j+1}^{[M]}$ is the final approximation after M corrector steps that we actually use. We can rewrite this as

$$y_{j+1}^{[l]} = \beta_{j+1} + \frac{h^\alpha}{\Gamma(\alpha+2)} f(x_{j+1}, y_{j+1}^{[l-1]}), \qquad (4.20)$$

where

$$\beta_{j+1} = \sum_{r=0}^{n-1} \frac{x_{j+1}^r}{r!} y_0^{(r)} + \frac{h^\alpha}{\Gamma(\alpha+2)} \sum_{r=0}^{j} a_{r,j+1} f(x_r, y_r), \qquad (4.21)$$

is independent of l. Thus the total arithmetic complexity of the corrector part of the $(j+1)$st step (taking us from x_j to x_{j+1}) is $O(j)$ for the calculation of β_{j+1} plus $O(M)$ for the M corrector steps, which is asymptotically the same as the complexity in the case $M = 1$. For the error of the scheme (4.20) and (4.21) we find by a repeated application of the considerations of the proof of Theorem 4.2.6 (see [41] for details).

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Theorem 4.2.8. Under the assumptions of Theorem 4.2.6, the approximation obtained by the $P(EC)^M E$ method described above satisfies

$$\max_{0 \le j \le N} |y(x_j) - y_j| = O(h^q)$$

where $q = \min\{2, 1 + M\alpha\}$.

(b) The second idea that we consider the fully implicit implementation of (4.10), with y_{k+1}^P replaced by y_{k+1}, in which y_{k+1} is computed by solving with Newton iteration to preserve the good stability properties for the nonlinear system

$$\Phi(y_{k+1}) - g_k = 0,$$

where

$$\Phi(y_{k+1}) \ := \ y_{k+1} - \frac{h^\alpha}{\Gamma(\alpha+2)} f(x_{k+1}, y_{k+1}),$$

$$g_k \ := \ \sum_{j=0}^{n-1} \frac{x_{k+1}^j}{j!} y_0^{(j)} + \frac{1}{\Gamma(\alpha)} \left(\sum_{j=0}^{k} a_{j,k+1} f(x_j, y_j) \right),$$

and for implementation, we need to work with the Jacobian of the right-hand side of the fractional differential equation .

(c) If $\alpha = 1$, the fractional Adams method (4.10) and (4.14) is reduced to the classical predictor-corrector method for first order differential equation (1.6)

$$y_{k+1}^P \ = \ y_k + h f(x_k, y_k),$$

$$y_{k+1} \ = \ \frac{h}{2} \left(f(x_k, y_k) + f(x_{k+1}, y_{k+1}^P) \right).$$

(d) In [136], a predictor-corrector algorithm was presented based on the generalized Taylor's formula, which is similar to (4.10) and (4.14), except that the predictor is chosen as

$$y_{k+1}^P = y_k + \frac{h^\alpha}{\Gamma(\alpha+1)} f(x_k, y_k). \tag{4.22}$$

The approximation (4.22) is commonly called the Generalized Euler Method (GEM)(that of course is an explicit method).

4.3 Examples

In the this section we are going to investigate the numerical methods described in Chapter 3 and Chapter 4 for two different problems.

Example 4.3.1. Consider the following linear FODE

$$^{C}D^{\alpha}y(x) = x^2 + \frac{2}{\Gamma(3-\alpha)}x^{2-\alpha} - y(x), \quad y(0) = 0, \quad 0 < \alpha \leq 1. \tag{4.23}$$

Its exact solution is given by

$$y(x) = x^2.$$

In this example, we test the approximations by means of the fractional backward differentiation methods by Grünwald-Letnikov (GL), Lubich with order $p = 2$ (Lp2) for $\alpha = 0.5$ and $\alpha = 0.1$ and various step sizes h. The resulting errors of the different schemes at $x = 1$ are shown in Table 4.1 for the case $\alpha = 0.5$ and $\alpha = 0.1$. We can find that the experimental (or estimation) order of convergence (EOC) of (GL) and (Lp2) are 1 and 2 respectively, which are in line with the theoretical analysis of Chapter 3. The EOC here is computed by the formula: $\log_2(\frac{E(h,X)}{E(h/2,X)})$, where the error $E(h, X) = |y(X) - y_{X/h}|$.

| | Errors at $x = 1$ | | | |
| | $\alpha = 0.5$ | | $\alpha = 0.1$ | |
$1/h$	GL	Lp2	GL	Lp2
10	3.06(-2)	1.24(-3)	2.74(-3)	
20	1.46(-2)	3.08(-4)	2.35(-3)	-4.49(-3)
40	7.11(-3)	7.86(-5)	1.27(-3)	-1.10(-3)
80	3.51(-3)	2.01(-5)	6.41(-4)	-2.76(-4)
160	1.75(-3)	5.15(-6)	3.20(-4)	-7.07(-5)
320	8.71(-4)	1.31(-6)	1.60(-4)	-1.83(-5)
640	4.35(-4)	3.33(-7)	8.00(-5)	-4.75(-6)
1280	2.17(-4)	8.43(-8)	3.99(-5)	-1.24(-6)
2560	1.09(-4)	2.12(-8)	2.00(-5)	-3.24(-7)
EOC	1.00	1.99	0.97	1.94

Table 4.1: Numerical results of the two BDF schemes for equation (4.23) with $\alpha = 0.5, 0.1$.

Example 4.3.2. Consider the following fractional differential equation

$$^{C}D^{\alpha}y(x) = -y(x) + \frac{x^{4-\alpha}}{\Gamma(5-\alpha)}, \quad 0 < \alpha < 1, \quad y(0) = 0, \quad x > 0. \tag{4.24}$$

its exact solution is

$$y(x) = x^4 E_{\alpha,5}(-x^{\alpha}),$$

where $E_{\alpha,\beta}(z)$ is the two-parameter Mittag-Leffler function (see Definition 1.2.10).

In this example, we apply the fractional Euler method (4.14) and the fractional Adams method to get the numerical solutions; the results are shown in Tables 4.2-4.3. The numerical results show good agreement with the exact solution. The long-term integration (10000 steps), i.e. the step-size $h = 1e - 5$, is tested in this example; the results are shown in Table 4.4, which shows good agreement with the analytical solutions.

$1/h$	$\alpha = 0.1$	$\alpha = 0.3$	$\alpha=0.5$	$\alpha=0.7$	$\alpha=0.9$
10	4.1205e-03	4.1397e-03	4.2821e-03	4.5571e-03	4.9388e-03
20	2.0192e-03	1.9788e-03	2.0515e-03	2.2207e-03	2.4550e-03
40	9.8557e-04	9.4634e-04	9.8894e-04	1.0892e-03	1.2222e-03
80	4.8052e-04	4.5427e-04	4.8032e-04	5.3731e-04	6.0937e-04
160	2.3428e-04	2.1912e-04	2.3490e-04	2.6625e-04	3.0416e-04
320	1.1429e-04	1.0623e-04	1.1553e-04	1.3235e-04	1.5192e-04
640	5.5794e-05	5.5794e-05	5.1741e-05	5.7071e-05	6.5923e-05

Table 4.2: The absolute errors at $x = 1$ for equation (4.24) by formula (4.14).

$1/h$	$\alpha = 0.1$	$\alpha = 0.3$	$\alpha=0.5$	$\alpha=0.7$	$\alpha=0.9$
10	8.3901e-03	2.8610e-03	1.4115e-03	8.3648e-04	5.6869e-04
20	4.0702e-03	1.0375e-03	4.4345e-04	2.3463e-04	1.4543e-04
40	1.7756e-03	3.7406e-04	1.4182e-04	6.7031e-05	3.7535e-05
80	7.4735e-04	1.3656e-04	4.6334e-05	1.9468e-05	9.7498e-06
160	3.1280e-04	5.0689e-05	1.5430e-05	5.7295e-06	2.5432e-06
320	1.3159e-04	1.9114e-05	5.2187e-06	1.7035e-06	6.6531e-07
640	5.5820e-05	7.3069e-06	1.7863e-06	5.1041e-07	1.7440e-07

Table 4.3: The absolute errors at $x = 1$ for equation (4.24) by the PECE method.

Methods	$\alpha = 0.3$	$\alpha=0.5$	$\alpha=0.8$
Euler method (4.14)	3.0345e-06	3.5706e-06	4.5247e-06
PECE method	5.0991e-07	2.7219e-08	1.8964e-09

Table 4.4: The absolute errors at $x = 1$ for equation (4.24) with $h = 1e - 5$.

Chapter 5

Fractional-order SIR models

In this chapter, two fractional order models are presented. The first one is the Susceptible-Infected-Recovered (SIR) model of a non-fatal disease in a population which is assumed to have a constant size over the period of the epidemic. The second one is the SIR model with variable size population which is formulated to include vaccination and treatment. The dynamics of such models are studied numerically by the methods described in Chapter 4.

5.1 The fractional order epidemic model of a non-fatal disease

We now consider the numerical solution of the fractional order epidemic model on long time intervals of a non-fatal disease in a population. Under real-life initial conditions the problem needs to be treated by means of an implicit numerical scheme (e.g. implicit fractional linear multistep methods of Adams type). Also, numerical results are presented.

5.1.1 Model description

In general, mathematical models of infectious a non-fatal diseases can provide important insight into our understanding of epidemiological processes, the course of infection within a host, the transmission dynamics in a host population, and formulation or implementation of infection control programs (see e.g. [20, 145, 146]). The model presented here can be used to model any infectious disease of humans or wildlife with discrete disease states, irrespective of the number of disease states.

The problem of spreading of a non-fatal disease in a population that is assumed to have constant size over the period of the epidemic can be formulated in terms of the following first order model (see [87, 88])

$$
\begin{cases}
S'(t) = -\beta S(t) I(t) \\[2mm]
I'(t) = \beta S(t) I(t) - \gamma I(t) \\[2mm]
R'(t) = \gamma I(t),
\end{cases}
\tag{5.1}
$$

with initial conditions

$$S(t_0) = N_1 \geq 0, \quad I(t_0) = N_2 \geq 0, \quad R(t_0) = N_3 \geq 0, \tag{5.2}$$

where at time $t \geq t_0$, $S(t)$ is the number of susceptible individuals, $I(t)$ is the number of infected individuals, able to spread the disease by contact with susceptible ones, $R(t)$ is the number of isolated individuals, who cannot get or transmit the disease for various reasons. Moreover, $\beta > 0$ is the rate of infection and $\gamma > 0$ is the rate at which current infective population is isolated. The non-fatality of the model (5.1) depends on the values of this two parameters. In Figure 5.2 we show an example of solution of (5.1) for small initial values.
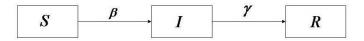

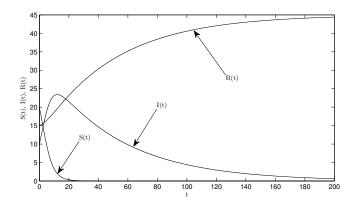Figure 5.1: Flowchart showing the compartment model for SIR.

Figure 5.2: Plots of numerical solutions for $S(t)$, $I(t)$, $R(t)$ versus time such that $N_1 = 20$, $N_2 = 15$, $N_3 = 10$, $\beta = 0.01$ and $\gamma = 0.02$.

The fractional order extension of this model have been first studied in [147], where the authors replace the first derivatives in (5.1) by Caputo's fractional derivative of order $0 < \alpha \leq 1$, defined by (see Definition 2.1.10 with $n = 1$),

$$_{t_0}^{C}D^{\alpha}f(t) = \frac{1}{\Gamma(1-\alpha)} \int_{t_0}^{t} (t-s)^{-\alpha} f'(s)ds, \tag{5.3}$$

The main reason that leads to this extension (typically with α chosen close to 1) is to reduce the error that may arise from neglected parameters or simplifications in the model (5.1), as for instance the choice of constant rate of infection β and isolation γ. This seems correct in principle

since this two parameters may change accordingly with the experience on the spreading of a certain epidemic, that is, on the history of the process. In this view, the use of $\alpha < 1$ has just the effect of transforming (5.1) into a model with memory. In general, the epidemic integer model (5.1)does not carry any information about the memory and learning mechanism of population that affects the spread of disease [156].

Without loss of generality, we assume that the process starts at time $t_0 = 0$. Then, using the simplified notation ${}^{C}_{0}D^{\alpha}f(t) = f^{(\alpha)}(t)$ we consider the numerical solution of the following fractional system of equations:

$$\begin{cases} S^{(\alpha)}(t) = -\beta S(t)I(t) \\[2mm] I^{(\alpha)}(t) = \beta S(t)I(t) - \gamma I(t) \\[2mm] R^{(\alpha)}(t) = \gamma I(t). \end{cases} \qquad (5.4)$$

Some of the recent analytic methods for solving nonlinear problems like (5.1) and (5.4) include the adomian decomposition method (ADM [20]), homotopy-perturbation method (HPM [146]), variational iteration method (VIM [145]) and homotopy analysis method (HAM [15] and [11, 147]). They are relatively new approaches to provide an analytical approximate solution to linear and nonlinear problems and they provide immediate and visible symbolic terms of analytic solutions. Anyway, such analytic methods are generally effective only for small time intervals.

Here we intend to solve (5.4) by discrete methods for FDEs, since we prefer to avoid restriction on the time interval under investigation. This may be important to forecast the end of the epidemic. Moreover, using real-life values for the initial conditions (5.2), problem (5.4) may become highly stiff and then it will be necessary to employ an implicit time-stepping scheme. In this situation, the use of analytic approximation by polynomials, attainable for instance by homotopy analysis method (HAM [11, 147]), seems unreliable.

5.1.2 Stability of the model

As mentioned in the previous subsection, assuming to work with real-life values for the initial conditions, the model (5.4) can be quite difficult to solve. Indeed, if we consider the Jacobian of the system,

$$J = \begin{pmatrix} -\beta I & -\beta S & 0 \\ \beta I & \beta S - \gamma & 0 \\ 0 & \gamma & 0 \end{pmatrix}, \qquad (5.5)$$

its nonzero eigenvalues are given by,

$$\lambda_{\pm} = \frac{1}{2}\left(\beta S - \gamma - \beta I\right) \pm \frac{1}{2}\sqrt{\left(\beta S - \gamma - \beta I\right)^2 - 4\beta\gamma I}.$$

Depending on the values assumed by S and I during the process, there is a negative eigenvalue that may be very large. In particular, the stationary point of the component I of the solution

(see Figure 5.2 and (5.4)), it is attained for $\beta S - \gamma = 0$, where $I > I_0$. In this situation,

$$\lambda_- = -\frac{\beta I}{2} - \frac{1}{2}\sqrt{\beta^2 I^2 - 4\beta\gamma I}.$$

In most of papers that considers the numerical results of this problem, the initial values and the parameters are taken such that $\beta I \approx 1$ or more generally very small. In this situation the problem can be solved efficiently by an explicit scheme since the eigenvalues remains close to the origin. Using more realistic (large) values for N_i, we clearly have that around the stationary point,

$$\lambda_- \approx -\beta I < -\beta N_2,$$

so that the problem needs to be solved by an implicit scheme.

5.1.3 Numerical results

In this subsection we present some numerical experiments for the model (5.4), using different values for the initial conditions. We consider relatively long time intervals and different values of α. In particular we work with $\alpha = 1, 0.99, 0.95$ represented respectively by a solid, dashed and dotted line in each figure. In Figure 5.3, for small initial conditions, we consider the Generalized Euler Method (GEM) given by formula (4.22). This method has been used in [12] for fractional order models of HTLV infection, in [13] to study the HIV during the primary infection and in [14] for the problem of the population dynamics of the human immunodeficiency type 1 virus (HIV-1).
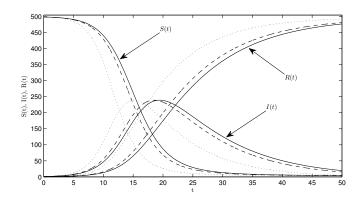

Figure 5.3: Numerical solutions by GEM for $N_1 = 499$, $N_2 = 1$, $N_3 = 1$ and $h = 0.01$ (see [15]).

In Figure 5.4 we plot the numerical solution given by the predictor corrector formula (4.10) and (4.14) for higher values of the initial conditions $N_1 = 10^4$, $N_2 = 10^3$ and $N_3 = 10$. We take $h = 0.01$ and apply only one corrector iteration. For this problem GEM produces unstable solutions unless we take $h = 0.001$. Using the same timestep $h = 0.01$, the predictor corrector formula shows a certain instability at the beginning of the process when $N_2 \geq 10^4$, as shown in

Figure 5.5. This phenomenon seems independent of the number of corrector iterations. The fully implicit implementation of (4.10) (see Remark 4.2.7 (b)) has been used to solve the problem with $N_1 = 10^5$, $N_2 = 10^4$ and $N_3 = 10^3$ (timestep $h = 0.01$). The results are shown in Figure 5.6.
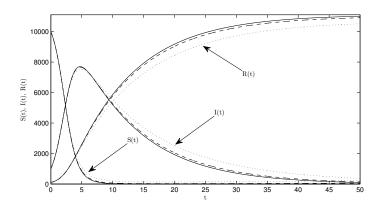

Figure 5.4: Numerical solutions by the PECE formula (4.10) and (4.14) with $N_1 = 10^4$, $N_2 = 10^3$, $N_3 = 10$ and $h = 0.01$.
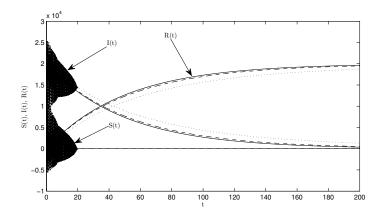

Figure 5.5: Numerical solutions by the $P(EC)^M E$ formula (4.20) and (4.21) with $N_1 = 10^4$, $N_2 = 10^4$, $N_3 = 10^2$ and $h = 0.01$. The number of corrector iterations $M = 2$.

5.1.4 Conclusion

In the last subsection we discussed numerical methods to obtain the solution of fractional epidemic model (5.4) over a long time period where HAM [11, 147] is not effective. Increasing the initial conditions the problem becomes difficult to solve. In particular, under realistic values of
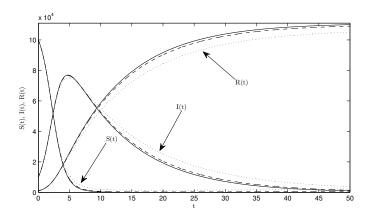
Figure 5.6: Numerical solutions for $S(t)$, $I(t)$, $R(t)$ versus time, where $N_1 = 10^5$, $N_2 = 10^4$ and $N_3 = 10^3$.

the initial conditions $N_1, N_2 \geq 10^4$, only the fully implicit formula is able to provide accurate solution with a reasonable choice of the timestep.

In the next section we also consider the fractional order SIR model but with, additional parameters, vaccination and treatment. It is important to note that this model is applicable to a class of diseases that is fatal, despite the availability of treatment and vaccination (e.g. *measles*).

5.2 The fractional order SIR model with vaccination and treatment

There are many of models for describing epidemics with different properties with respect to mortality, immunity, time horizon and so on (e.g. [65, 134, 167, 177, 180]). Here, one of these models is examined. Precisely, we considered a standard SIR model with vaccination, treatment and variable total population. We show that this model possesses non-negative solutions as desired in any population dynamics. Also, the stability of equilibrium points is studied. Graphical results are presented and discussed.

5.2.1 Model description

To derive this model we suppose the total population $N(t)$ is partitioned into three compartments which are Susceptible $S(t)$, Infectious $I(t)$ and Recovered $R(t)$. Let b denote the birth (recruitment) rate of the population, β is the disease transmission rate between infected and susceptible. We assume d to be the natural death rate, σ is the disease-induced death rate. Also, we assume there exists μ_1 and μ_2 which respectively denotes the proportion of the susceptible that is vaccinated per unit time and the proportion of the infectives that is treated per unit
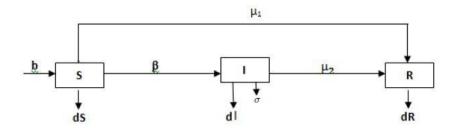
time.

Figure 5.7: Flowchart showing the compartment model for SIR with μ_1 and μ_2.

The assumptions of the model leads to the following system of ODEs

$$
\begin{cases}
S'(t) = b - \beta S(t)I(t) - (d + \mu_1)S(t), \\[2mm]
I'(t) = \beta S(t)I(t) - (\mu_2 + d + \sigma)I(t), \\[2mm]
R'(t) = \mu_1 S(t) + \mu_2 I(t) - dR(t).
\end{cases}
\tag{5.6}
$$

The total population $N(t)$ can be obtained from $N(t) = S(t) + I(t) + R(t)$ or, by adding the right-side of (5.6), we have

$$
N'(t) = b - d\,N(t) - \sigma I(t).
$$

This means that the population size is not constant (i.e. variable size population). Since $R(t)$ can always be obtained by the equation $R(t) = N(t) - S(t) - I(t)$. So, we have the following system

$$
\begin{cases}
S'(t) = b - \beta S(t)I(t) - (d + \mu_1)S(t), \\[2mm]
I'(t) = \beta S(t)I(t) - (\mu_2 + d + \sigma)I(t), \\[2mm]
N'(t) = b - d\,N(t) - \sigma I(t),
\end{cases}
\tag{5.7}
$$

under initial conditions

$$
S(t_0) = S_0, \quad I(t_0) = I_0, \quad N(t_0) = N_0.
\tag{5.8}
$$

Now we introduce the fractional-order system of (5.7), where $D^\alpha S$, $D^\alpha I$ and $D^\alpha N$ are the derivatives of $S(t)$, $I(t)$, and $N(t)$ respectively, of arbitrary order α (where $0 < \alpha < 1$) in the sense of Caputo (5.3), then the new system is described by the following set of fractional order differential equations

$$
\begin{cases}
D^\alpha S(t) = b - \beta S(t)I(t) - (d + \mu_1)S(t), \\[2mm]
D^\alpha I(t) = \beta S(t)I(t) - (\mu_2 + d + \sigma)I(t), \\[2mm]
D^\alpha N(t) = b - d\,N(t) - \sigma I(t),
\end{cases}
\tag{5.9}
$$

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subject to the same initial conditions given in (5.8). The main reason that leads to this extension (typically with α chosen close to 1) is to reduce the error that may arise from neglected parameters or simplifications in the model (5.7). When a disease outbreak occur, the predicted number of individuals who are infected and recovered due to the vaccination by the model (5.7) might be significantly different (less or more) than the realistic data. Hence the fractional model (5.9) possess memory. So, we will use the fractional order (where memory effects are important) model (5.9) in order to analyze and evaluate the disease.

We intend to solve the model (5.9) by formula (4.14), which offer accurate solution during a long time interval. This may be important in order to show the effect of vaccination μ_1 and treatment μ_2 of the fractional order model (5.9).

5.2.2 Non-negative solutions

Let $\mathbb{R}^3_+ = \{X \in \mathbb{R}^3 | X \geq 0\}$ and $X(t) = (S(t), I(t), N(t))^T$, we now prove the main theorem.

Theorem 5.2.1. *There is a unique solution $X(t) = (S(t), I(t), N(t))^T$ for model (5.9) at $t \geq 0$ (where, $t_0 = 0$) and the solution will remain in $\mathbb{R}^3_+$.*

Proof. From Theorem 3.1 and Remark 3.2 of [100], we know that the solution on $(0, \infty)$ is existent and unique. Now, we will show that the feasible region $\mathbb{R}^3_+$ is positively invariant (non-negative solutions). Rearranging the last equation for the system (5.9) and we assume that $f(t) = b - \sigma I$ is a constant function of time. Then we get the fractional order differential equation representing the total population as follows:

$$D^\alpha N(t) + d \ N(t) = f(t). \tag{5.10}$$

Solving equation (5.10) using Laplace transform method [141] (see Table 2.1 for $\mathscr{L}\{^C D^\alpha N(t)\}$) and taking the initial condition to be zero (to simplify), we have the following solution

$$N(t) = \int_0^t (t - \tau)^{\alpha-1} E_{\alpha,\alpha}(-d \ (t - \tau)^\alpha) f(\tau) d\tau \ \geq 0,$$

where $0 < \alpha < 1$, $d > 0$ and $E_{a,b}(z)$ is the two-parameter Mittag-Leffler function (see Definition 1.2.10). Since Mittag-Leffler function is an entire function [141] thus $E_{\alpha,\alpha}(-d(t-\tau)^\alpha)$ is bounded for all $t > 0$. Therefore, as $k \to \infty$ and $t \to \infty$, we have $N \leq \frac{b}{d}$. For $S(t)$, $I(t)$ by the same way we have $S(t) \geq 0$ and $I(t) = 0$, hance proved that the solution $X(t)$ is positive invariant. $\square$

5.2.3 Equilibrium points and their asymptotic stability

To determine the stability analysis, we first evaluate the equilibrium points or steady states of the system (5.9). The equilibrium points involved determine the disease-free (where $I = 0$) and endemic (where $I \neq 0$).

To evaluate the equilibrium points, let

$$\begin{cases} D^\alpha S = 0, \\ D^\alpha I = 0, \\ D^\alpha N = 0, \end{cases} \tag{5.11}$$

then, the system (5.9) has two equilibrium points

1. *At disease-free equilibrium:*

   We now consider the equations below and solve for the values S and N, since at this point there is no infection, thus from (5.11)

   $$b - \beta SI - (d + \mu_1)S = 0, \tag{5.12}$$

   $$\beta SI - (\mu_2 + d + \sigma)I = 0, \tag{5.13}$$

   $$b - dN - \sigma I = 0. \tag{5.14}$$

   From equation (5.13), we have $I = 0$, then by substituting in equations (5.12), (5.14). Then disease-free equilibrium (DFE) of the system (5.9) is

   $$\varepsilon_1 = (S_{eq}, I_{eq}, N_{eq})_{I=0} = \left(\frac{b}{d + \mu_1}, \ 0, \ \frac{b}{d} \right).$$

   Using the next-generation operator approach [48, 171], we derive the expression of the basic reproduction number $\mathcal{R}_0$ (see Subsection 2.3.4), allied to the DFE (i.e. ε_1). Following, [48, 171], the next generation matrix is given by (FV^{-1}). Then, we can compute the basic reproduction number as follow:

   $$\mathcal{R}_0 = \rho(FV^{-1}),$$

   where ρ denotes the eigenvalue of largest magnitude or spectral radius. First, we re-order the system of equation (5.9) to get

   $$\begin{aligned} f_1(I, S, N) &= \beta SI - (\mu_2 + d + \sigma)I, \\ f_2(I, S, N) &= b - \beta SI - (d + \mu_1)S, \\ f_3(I, S, N) &= b - dN - \sigma I. \end{aligned}$$

   Linearization of the above system gives the generation matrix (G) evaluated at the DFE,

   $$G = \begin{bmatrix} f_1 I & f_1 S & f_1 N \\ f_2 I & f_2 S & f_2 N \\ f_3 I & f_3 S & f_3 N \end{bmatrix}.$$

Since f_1 and f_2 form a subsystem describing the generation and transition of infectious, the Jacobian matrix associated with the linearized subsystem at DFE is given by,

$$J_{DFE}(I,S) = \begin{bmatrix} \beta S_{eq} - (\mu_2 + d + \sigma) & 0 \\ -\beta S_{eq} & -(d + \mu_1) \end{bmatrix}.$$

J_{DFE} is decomposed as $F - V$, where the non-negative matrix F, representing the matrix of new infection and the non-singular matrix V, representing transmission term of different infected compartments of the model (5.9), i.e.

$$F = \begin{bmatrix} \beta S_{eq} & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad V = \begin{bmatrix} \mu_2 + d + \sigma & 0 \\ \beta S_{eq} & (d + \mu_1) \end{bmatrix}.$$

Thus, the next generation matrix becomes

$$FV^{-1} = \begin{bmatrix} \frac{b\beta}{(d+\mu_1)(\mu_2+d+\sigma)} & 0 \\ 0 & 0 \end{bmatrix},$$

where we have $S_{eq} = \frac{b}{d+\mu_1}$ at DFE. Since $\mathcal{R}_0 = \rho(FV^{-1})$, then

$$\mathcal{R}_0 = \frac{b\beta}{(d + \mu_1)(\mu_2 + d + \sigma)}. \tag{5.15}$$

2. *At endemic equilibrium:*

We now consider the case where there is infection, thus from equation (5.13) $S = \frac{\mu_2+d+\sigma}{\beta}$ by substituting in equations (5.12) and (5.14), then we have

$$\varepsilon_2 = (S_{eq}, I_{eq}, N_{eq})_{I\neq 0} = (S^*, I^*, N^*)$$

where

$$S^* = \frac{\mu_2 + d + \sigma}{\beta},$$

$$I^* = (\mathcal{R}_0 - 1)\frac{\mu_1 + d}{\beta},$$

$$N^* = \frac{b\beta(\mu_2 + d) + \sigma(\mu_1 + d)(\mu_2 + d + \sigma)}{d\beta(\mu_2 + d + \sigma)}.$$
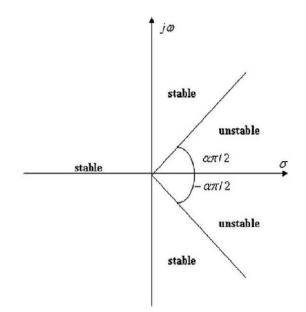
100

Figure 5.8: Stability region of the fractional-order system.

We can note that the equilibrium points are the same for both integer and fractional system. But the stability region of the fractional-order system with order α, which is illustrated in Figure 5.8 (where σ, ω refer to the real and imaginary parts of the eigenvalues, respectively, and $j = \sqrt{-1}$), is gearter than the stability region of the integer order case (see e.g.[56]). Therefore, we will now drive analytically the stability of different equilibria of the model (5.9).

For ε_1, ε_3 and the expression (5.15) of $\mathcal{R}_0$, we have the following theorems:

Theorem 5.2.2. *The disease free equilibria ε_1 of the system (5.9) is locally asymptotically stable if $\mathcal{R}_0 < 1$.*

Proof. Determining the Jacobian matrix of the system (5.9) at ε_1 we have:

$$
J_{\varepsilon_1} = \begin{bmatrix} -d - \mu_1 & \frac{-b\beta}{d+\mu_1} & 0 \\ 0 & \frac{b\beta}{d+\mu_1} - \mu_2 - d - \sigma & 0 \\ 0 & -\sigma & -d \end{bmatrix}.
$$

The eigenvalues of J_{ε_1} are

$$
\lambda_1 = -(d + \mu_1) < 0, \ \lambda_3 = -d < 0, \ \lambda_2 = \frac{b\beta}{d + \mu_1} - (\mu_2 + d + \sigma).
$$

Now, we should give the following remark to continue with our proof.

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Remark 5.2.3. Disease free equilibrium ε_1 of the system (5.9) is locally asymptotically stable if $|\arg(\lambda_i)| > \frac{\alpha\pi}{2}$, $\forall\, i = 1, 2, 3$ (see e.g. [5, 57]).

If $\mathcal{R}_0 = \frac{b\beta}{(d+\mu_1)(\mu_2+d+\sigma)} < 1$, then $\frac{b\beta}{d+\mu_1} < (\mu_2 + d + \sigma) \Rightarrow \lambda_2 < 0$ and therefore, $|\arg(\lambda_i)| > \frac{\alpha\pi}{2}$, $\forall\, i = 1, 2, 3$. Thus, disease free equilibrium ε_1 of the system (5.9) is locally asymptotically stable if $\mathcal{R}_0 < 1$. $\qquad\qquad\square$

Theorem 5.2.4. *The endemic equilibrium point ε_2 is locally asymptotically stable if $\mathcal{R}_0 > 1$.*

Proof. The Jacobian matrix evaluated at the endemic equilibrium gives

$$
J_{\varepsilon_2} = \begin{bmatrix} -\mathcal{R}_0(\mu_1 + d) & -(d + \mu_2 + \sigma) & 0 \\[2mm] (\mathcal{R}_0 - 1)(\mu_1 + d) & 0 & 0 \\[2mm] 0 & -\sigma & -d \end{bmatrix}
$$

and its eigenvalues are

$$
\lambda_1 = -d < 0, \ \ \lambda_{2,3} = \frac{-\mathcal{R}_0(\mu_1 + d) \pm \sqrt{\mathcal{R}_0^2(\mu_1 + d)^2 - 4(\mathcal{R}_0 - 1)(\mu_1 + d)(d + \mu_2 + \sigma)}}{2}.
$$

This shows that if $\mathcal{R}_0 > 1$, then $\lambda_2 < 0$ and $\lambda_3 < 0$, hence it becomes asymptotically stable. $\quad\square$

5.2.4 Numerical results

We are now going to study the effect of vaccination μ_1 and treatment μ_2 on the dynamics of the disease described by the fractional-order model (5.9), using the formula (4.14). The following values, for parameters (see [179]), are considering

$$b = 0.03, \quad d = 0.02, \quad \sigma = 0.1, \quad \beta = 0.75, \quad S_0 = 0.95, \quad I_0 = 0.05, \quad N_0 = 1. \qquad (5.16)$$

From this values of parameters, we estimate that $\mathcal{R}_0 = \frac{0.0225}{(\mu_1 + 0.02)(\mu_2 + 0.12)}$. The approximate solutions displayed in Figures 5.9-5.11 for step-size $h = 0.1$ with different value of fractional order $0 < \alpha \leq 1$ and it is clear that varying the values of μ_1 and μ_2 will alter the number of susceptible and infected persons. If $\mu_1 = \mu_2 = 0$ (i.e. in the absence of vaccination and treatment), then $\mathcal{R}_0 = 9.3750 > 1$ and from the results the disease will persist, while in the beginning of time interval the number of susceptible decrease (see Figure 5.9(a)), the number of infected increases (see Figure 5.9(b)) and in Figure 5.9(c) we can note that $N(t)$ never goes to extinction, this is the main reason for chosen these values of parameters (5.16). If $\mu_1 = \mu_2 = 1$ (i.e. in the presence of vaccination and treatment), $\mathcal{R}_0 = 0.0197 < 1$, the number of susceptible dramatically decreased due to the population have been already vaccinated (see Figure 5.11(a)) and the infection will die out (see Figure 5.11(b)). About the relevance of vaccination and treatment is obvious from Figure 5.10. For the fractional order case, in Figure 5.9(b) the climax of $I(t)$ is reduced. But the disease takes a longer time to be eradicated (see Figure 5.11(b)). From the numerical results in Figures 5.9-5.11, it is clear that the approximate solutions continuously depends on the time-fractional derivative α.
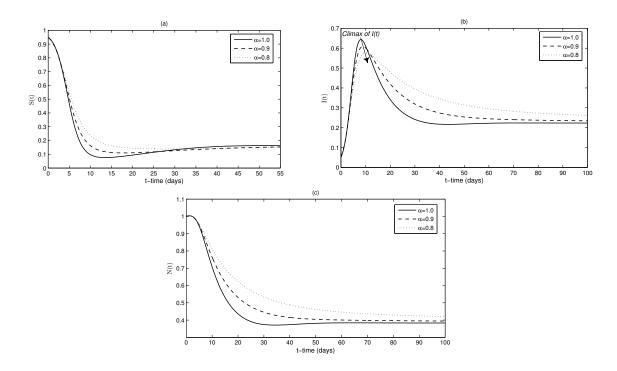
Figure 5.9: (a) $S(t)$, (b) $I(t)$, (c) $N(t)$ versus t with different values of α and $\mathcal{R}_0 > 1$.
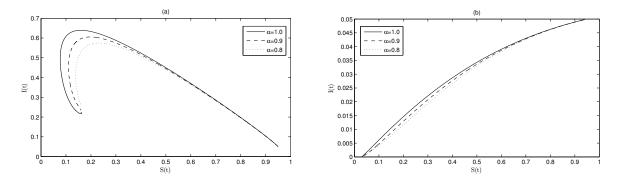

Figure 5.10: $I(t)$ versus $S(t)$ with different values of α where (a) $\mathcal{R}_0 > 1$ and (b) $\mathcal{R}_0 < 1$.

5.2.5 Conclusion

In Section 5.2 we have been able to extend the ODE model (5.7) to take care of all the properties and also the principle of the proposed model (5.9) possess memory. We obtained the non-negative solutions of the fractional model by Laplace transform method. We carried out numerical solutions to verify the theoretical analysis by applying the fractional Euler method (4.14). The numerical results confirmed that in the absence of vaccination and treatment the disease persists while in the presence of vaccination and treatment the disease die out. We need
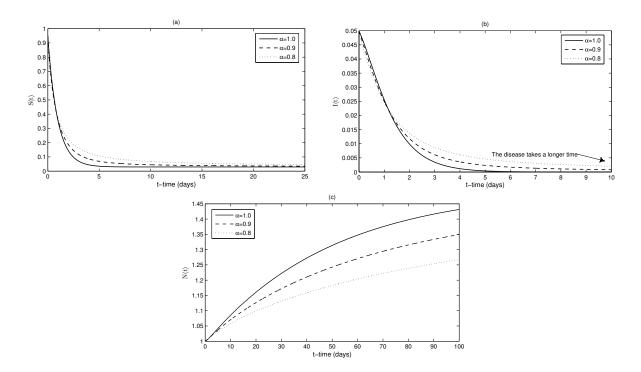
Figure 5.11: (a) $S(t)$, (b) $I(t)$, (c) $N(t)$ versus t with different values of α and $\mathcal{R}_0 < 1$.

to mention that when dealing with epidemic diseases in a population, the order of the fractional system can be determined by using the collected data.

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