Numerical Approximation of Spike-Type Solutions to a One-Dimensional Sub-Diffusive Gierer-Meinhardt Model with Controlled Precision.

by

Nehemie Nguimbous

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We accept this thesis as conforming to the required standards:

Yana Nec
Supervisor's Name
Dept. of Mathematics & Statistics
Thesis Supervisor

Shirin Boroushaki
First Examiner's Name
Dept. of Mathematics & Statistics

Richard Brewster
Second Examiner's Name
Dept. of Mathematics & Statistics

Dated April 8 2024, Kamloops, British Columbia, Canada

THOMPSON RIVERS UNIVERSITY
DEPARTMENT OF MATHEMATICS & STATISTICS

Signature of Author

Abstract

This thesis focuses on numerically solving the sub-diffusive Gierer-Meinhardt model with controlled precision. We start by defining and explaining basic concepts of reaction diffusion, highlighting the main differences between normal and anomalous diffusion. Sub-diffusion is modelled at continuum level by fractional derivatives replacing regular ones in PDEs. Therefore a crucial part of our study involves fractional calculus, which provides a solid framework for describing subdiffusive processes. We explore integer and fractional derivatives and integrals, their main properties, those that can be extended from classical to fractional calculus, and the reasons for limitations in some cases.

We then delve into the well-known Gierer-Meinhardt model, a reaction-diffusion system used to describe pattern formation in biological systems. Leveraging the matched asymptotic expansion technique, which is applicable due to the asymptotic smallness of certain parameters in the system, we transform the differential Gierer-Meinhardt model into a differintegro-algebraic system.This differintegro-algebraic system contains a fractional operator denoted $\mathcal{D}_t^\gamma$, which involves the integral of a complex function impossible to determine analytically. This operator depends on multiple parameters, and the number of subdivisions needed for numerical computation varies significantly with these parameters and the desired precision. To address this challenge, we have developed a program capable of precalculating the required number of subdivisions before computation, thus saving significant computation time. All elements in place, we use these tools to study the dynamics of the obtained spikes.

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Contents

Chapter 1

Reaction-Diffusion

Definitions and Types

Reaction-diffusion is a dynamic process in which the spatial distribution of chemical substances evolves over time due to the interplay between those chemicals and their diffusion through space. The system typically involves an "activator," a chemical component that promotes its own production and that of other substances. Simultaneously, an "inhibitor" is present, which suppresses its own production and that of other substances. The delicate balance between the concentrations of the activator and the inhibitor, along with their diffusion properties, gives rise to intricate patterns and structures such as stripes, spots, and spikes. These patterns are observed in various animals' skins, such as zebras, cheetahs, or giraffes. Moreover, reaction-diffusion is also responsible for the regulation that must take place during organism growth, such as the formation of new tissue.

Types of Diffusion

Depending on specific system parameters and conditions, we can distinguish between two main types of diffusion: normal and anomalous diffusion.

1. Normal diffusion: is characterized by Fick's law:

$$J = -D\nabla C,$$

   where J represents the diffusion flux, D the diffusion coefficient, and C the concentration of the substance. This process involves the random linear movement of particles from regions of higher concentration to lower concentration. The mean square displacement of the particles is expressed as a linear function of time.

$$r^2(t) \sim t.$$

2. Anomalous diffusion is characterized by a non-linear displacement of particles. The mean square displacement of the particles is expressed as a power function of time:

$$r^2(t) \sim t^{\gamma}.$$

There exist two main types of anomalous diffusion: sub-diffusion and super-diffusion. The former occurs when the spread of particles is slower than that of normal diffusion, characterized by $\gamma < 1$, while the latter arises when the displacement of the particles is faster, with $\gamma > 1$.

Chapter 2

Classical and Fractional Calculus

2.1 Background, Properties, Similarities and Differencies

This section is based in its entirety on the textbook [7]. The main topic of the text is to generalise integer derivatives and integrals to fractional orders. Before embarking on this journey, an auxiliary topic needed throughout the book is the Γ function, distinguished by its extensive usage throughout the text and its significant contributions to key results. The Γ function, defined as

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

and it has several fundamental properties, including:

1. **Factorial Property**: For a positive integer n, $\Gamma(n) = (n-1)!$.
2. **Recurrence Relation**: $\Gamma(z+1) = z\Gamma(z)$.
3. **Reflection Formula**: $\Gamma(z)\Gamma(1-z) = \dfrac{\pi}{\sin(\pi z)}, \quad z \notin \mathbb{Z}$.
4. **Euler's Identity**: $\Gamma(z) = \lim\limits_{n\to\infty} \dfrac{n^z n!}{z(z+1)\cdots(z+n)}$.
5. **Duplication Formula**: $\Gamma(2z) = 2^{2z-1}\Gamma(z)\Gamma\left(z+\dfrac{1}{2}\right)\dfrac{1}{\sqrt{\pi}}$.
6. **Asymptotic expansion**:

$$\frac{\Gamma(j-q)}{\Gamma(j+1)} \sim j^{-1-q}\left[1 + \frac{q[q+1]}{2j} + \mathcal{O}(j^{-2})\right], \quad q \in \mathbb{R}, \quad j \in \mathbb{N}, \quad \text{and} \quad j \to \infty. \tag{2.1}$$

A function that is closely related to the Gamma function is the Beta function $\mathrm{B}(p,q)$. For positive values of the two parameters, p and q, the function is defined by the Beta integral

$$\mathrm{B}(p,q) = \int_0^1 y^{p-1}[1-y]^{q-1}dy, \quad p > 0 < q, \tag{2.2}$$

also known as Euler's integral of second kind. If either p or q is non-positive, the integral diverges and the Beta function is defined by the relationship

$$\mathrm{B}(p,q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}. \tag{2.3}$$

2.1.1 Classical or Integer Calculus

Integer calculus, commonly known as classical calculus, has its origins deeply rooted in the monumental contributions of Isaac Newton and Gottfried Wilhelm Leibniz during the 17th century. These mathematical pioneers independently developed the fundamental principles of differentiation and integration, forming the bedrock of classical calculus. Hereinafter we will review the classical notions of differentiation and integration with the view to unify them as one overarching concept and from there generalise to a non-integer order.

Integer Derivative

In classical calculus, the derivative of a function represents the rate at which the function's output changes with respect to its input. The first order integer derivative is defined as

$$\frac{d^1 f(x)}{[d(x-a)^1]} = \frac{df(x)}{d(x-a)} = \lim_{\delta x \to 0}\left\{\Big[\delta x\Big]^{-1}\Big[f(x) - f(x-\delta x)\Big]\right\}, \tag{2.4}$$

where $\delta x = \dfrac{x-a}{N}$, with a being an immaterial real number less than x and N being a positive integer greater or equal to 1. Subsequently, the second order integer derivative, ensued by applying the derivative once to (2.4) is defined as

$$\frac{d^2 f(x)}{[d(x-a)^2]} = \lim_{\delta x \to 0}\left\{\Big[\delta x\Big]^{-2}\Big[f(x) - 2f(x-\delta x) + f(x-2\delta x)\Big]\right\}. \tag{2.5}$$

In the same way, the third order integer derivative is defined as

$$\frac{d^3 f(x)}{[d(x-a)^3]} = \lim_{\delta x \to 0}\left\{\Big[\delta x\Big]^{-3}\Big[f(x) - 3f(x-\delta x) + 3f(x-2\delta x) - f(x-3\delta x)\Big]\right\}. \tag{2.6}$$

The n^{th} order integer derivative is generalized as follows

$$\frac{d^n f(x)}{[d(x-a)^n]} = \lim_{\delta x \to 0}\left\{\Big[\delta x\Big]^{-n}\sum_{j=0}^{n}\Big[-1\Big]^{j}\binom{n}{j} f(x-j\,\delta x)\right\}. \tag{2.7}$$

Integer Integration or Antidifferentiation

The integral of a function represents the accumulation of a quantity described by the function over an interval. Geometrically, it corresponds to the area under the curve of the function in a given interval. Because integration and differentiation are inverse operations, it is natural to unify their symbolism. Using the definition of an integral as a limit of a Riemann sum, we have

$$\begin{aligned}\frac{d^{-1}f(x)}{[d(x-a)^{-1}]} &= \int_a^x f(t)\,dt = \lim_{\delta x\to 0}\left\{\Big[\delta x\Big]\Big[f(x)+f(x-\delta x)+f(x-2\delta x)+\ldots+f\Big(x-(N-1)\delta x\Big)\Big]\right\}\\ &= \lim_{\delta x\to 0}\left\{\Big[\delta x\Big]\sum_{j=0}^{N-1} f(x-j\ \delta x)\right\}.\end{aligned} \tag{2.8}$$

Applying the same definition to a double integration leads to

$$\begin{aligned}\frac{d^{-2}f(x)}{[d(x-a)^{-2}]} &= \int_a^x\int_a^{x_1} f(t)\,dt\ dx_1\\ &= \lim_{\delta x\to 0}\left\{\Big[\delta x\Big]^2\Big[f(x)+2f(x-\delta x)+3f(x-2\delta x)+\ldots+Nf\Big(x-(N-1)\delta x\Big)\Big]\right\}\\ &= \lim_{\delta x\to 0}\left\{\Big[\delta x\Big]^2\sum_{j=0}^{N-1}\Big[j+1\Big]f(x-j\ \delta x)\right\}.\end{aligned} \tag{2.9}$$

We need to integrate one more time to get a better grasp of the overall formula:

$$\frac{d^{-3}f(x)}{[d(x-a)^{-3}]} = \int_a^x\int_a^{x_2}\int_a^{x_1} f(t)\,dt\ dx_1\ dx_2 \quad = \lim_{\delta x\to 0}\left\{[\delta x]^3\sum_{j=0}^{N-1}\frac{[j+1][j+2]}{2}f(x-j\ \delta x)\right\}. \tag{2.10}$$

This time, we observe that the coefficients accumulate as $\begin{pmatrix} j+n-1\\ j\end{pmatrix}$, with n representing the integral's order, and all coefficients are positive. Hence,

$$\frac{d^{-n}f(x)}{[d(x-a)^{-n}]} = \lim_{\delta x\to 0}\left\{\Big[\delta x\Big]^n\sum_{j=0}^{N-1}\begin{pmatrix} j+n-1\\ j\end{pmatrix}f(x-j\ \delta x)\right\}. \tag{2.11}$$

Matching of the Differentiation and Integration Expressions: Differintegration

Using the convention that $\binom{n}{j} = 0$ when $j > n$, with both numbers integers, equation (2.7) can be reformulated as:

$$\frac{d^n f(x)}{[d(x-a)^n]} = \lim_{\delta x \to 0} \left\{ \Big[\delta x\Big]^{-n} \sum_{j=0}^{N-1} \Big[-1\Big]^j \binom{n}{j} f(x - j\ \delta x) \right\}, \tag{2.12}$$

where $N - 1 > n$. This convention is consistent with the Γ function interpretation, since Γ of a negative integer is infinite. By comparing formulas (2.7) and (2.11), and recalling that

$$\Big[-1\Big]^j \binom{n}{j} = \binom{j-n-1}{j} = \frac{\Gamma(j-n)}{\Gamma(-n)\Gamma(j+1)},$$

equations (2.7) and (2.11) can be unified in the following equation:

$$\frac{d^q f(x)}{[d(x-a)^q]} = \lim_{\delta x \to 0} \left\{ \frac{[\delta x]^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x - j\ \delta x) \right\}, \tag{2.13}$$

with q being an integer of either sign. Note that for a positive q the expression $\Gamma(-q)$ is infinite, but for $j \le q$ within the sum the infinite $\Gamma(j-q)$ divided by $\Gamma(j+1)$ will together give a finite value after using the recursion formula for the Gamma function. For all other $j > q$ the factor $\Gamma(-q)$ will nullify the contribution.

Composition Rule

For positive integers, we have

$$\frac{d^n}{[d(x-a)^n]} \left\{ \frac{d^N f(x)}{[d(x-a)^N]} \right\} = \frac{d^N}{[d(x-a)^N]} \left\{ \frac{d^n f(x)}{[d(x-a)^n]} \right\} = \frac{d^{n+N} f(x)}{[d(x-a)^{n+N}]}(x). \tag{2.14}$$

For negative integers, we have

$$\frac{d^{-n}}{[d(x-a)^{-n}]} \left\{ \frac{d^{-N} f(x)}{[d(x-a)^{-N}]} \right\} = \frac{d^{-N}}{[d(x-a)^{-N}]} \left\{ \frac{d^{-n} f(x)}{[d(x-a)^{-n}]} \right\} = \frac{d^{-n-N} f(x)}{[d(x-a)^{-n-N}]}. \tag{2.15}$$

However, a problem arises when it comes to mixed composition. In fact, we will show that in some cases, for orders of opposite signs the composition is not commutative.

On one hand, let us adopt the notation $\frac{d^N f(x)}{[d(x-a)^N]} = f^N(x)$ with N a positive integer.
For $n = 1$ we have

$$\frac{d^{-1} f^{(N)}(x)}{[d(x-a)^{-1}]} = \int_a^x f^{(N)}(x) dx = f^{(N-1)}(x) - f^{(N-1)}(a).$$

For $n = 2$ we have

$$\frac{d^{-2}f^{(N)}(x)}{[d(x-a)^{-2}]} = \int_a^x \left(f^{(N-1)}(x) - f^{(N-1)}(a)\right) dx = f^{(N-2)}(x) - f^{(N-2)}(a) - (x-a)f^{(N-1)}(a). \tag{2.16}$$

Based on the expressions for different values of n, the general expression for any positive integer n is

$$\frac{d^{-n}f^{N}(x)}{[d(x-a)^{-n}]} = f^{(N-n)}(x) - \sum_{k=0}^{n-1} \frac{[x-a]^k}{k!} f^{[N+k-n]}(a). \tag{2.17}$$

On the other hand, by substituting $N = 0$ in (2.17), we have

$$\frac{d^{-n}f(x)}{[d(x-a)^{-n}]} = f^{(-n)}(x) - \sum_{k=0}^{n-1} \frac{[x-a]^k}{k!} f^{(k-n)}(a). \tag{2.18}$$

Upon differentiating (2.18) once we have

$$\frac{d}{[d(x-a)]}\left\{\frac{d^{-n}f(x)}{[d(x-a)^{-n}]}\right\} = f^{(1-n)}(x) - \sum_{k=1}^{n-1} \frac{[x-a]^{k-1}}{(k-1)!} f^{(k-n)}(a).$$

After N such differentiations, the equation

$$\frac{d^N}{[d(x-a)^N]}\left\{\frac{d^{-n}f(x)}{[d(x-a)^{-n}]}\right\} = f^{(N-n)}(x) - \sum_{k=N}^{n-1} \frac{[x-a]^{k-N}}{(k-N)!} f^{(k-n)}(a)$$

emerges. This expression encompasses the case $N \geq n$ where $\sum_{k=N}^{n-1} \frac{[x-a]^{k-N}}{(k-N)!} f^{(k-n)}(a) = 0$ and the case $N < n$. Finally, we have established that

$$\begin{aligned}
\frac{d^N}{[d(x-a)^N]}\left\{\frac{d^{-n}f(x)}{[d(x-a)^{-n}]}\right\} &= f^{(N-n)}(x) - \sum_{k=N}^{n-1} \frac{[x-a]^{k-N}}{(k-N)!} f^{(k-n)}(a) \\
&= f^{(N-n)}(x) - \sum_{k=0}^{n-1-N} \frac{[x-a]^{k}}{k!} f^{(k-n+N)}(a) \\
&= f^{(N-n)}(x) - \sum_{k=0}^{n-1} \frac{[x-a]^{k}}{k!} f^{(k-n+N)}(a) \\
&+ \sum_{k=n-N}^{n-1} \frac{[x-a]^{k}}{k!} f^{(k-n+N)}(a) \\
&= \frac{d^{-n}f^{N}(x)}{[d(x-a)^{-n}]} + \sum_{k=n-N}^{n-1} \frac{[x-a]^{k}}{k!} f^{(k-n+N)}(a).
\end{aligned} \tag{2.19}$$

In summary, the composition rule $\frac{d^q}{[d(x-a)^q]}\left\{\frac{d^Q f(x)}{[d(x-a)^Q]}\right\} = \frac{d^{q+Q} f(x)}{[d(x-a)^{q+Q}]}(x)$ holds unless Q is positive and q is negative. In other words, unless f is first differentiated and then integrated. In this case the equality holds only if $f(a) = 0$ and if all derivatives of f through the $(N-1)^{th}$ are also zero at $x = a$.

Product Rule for Multiple Integrals

In this section our focus is on establishing a rule for iterated integration of a product of two functions, akin to Leibniz's theorem for repeated differentiation of a product. To initiate this process, we start with the well-known formula of integration by parts

$$\int_a^x g(y)dv(y) = g(x)v(x) - g(a)v(a) - \int_a^x v(y)dg(y). \tag{2.20}$$

Let

$$v(y) = \int_a^y f(z)dz,$$

then

$$\int_a^x g(y)f(y)dy = g(x)\int_a^x f(z)dz - \int_a^x \Big[\int_a^y f(z)dz\Big]\frac{dg(y)}{dy}dy, \tag{2.21}$$

or in the previous symbolism we have

$$\frac{d^{-1}[fg]}{[d(x-a)]^{-1}} = g\frac{d^{-1}f}{[d(x-a)]^{-1}} - \frac{d^{-1}}{[d(x-a)]^{-1}}\left\{g^{(1)}\frac{d^{-1}f}{[d(x-a)]^{-1}}\right\}. \tag{2.22}$$

Upon applying (2.22) recursively to the product within the braces and invoking the composition rule, we obtain:

$$\begin{aligned}\frac{d^{-1}[fg]}{[d(x-a)]^{-1}} &= g\frac{d^{-1}f}{[d(x-a)]^{-1}} - g^{(1)}\frac{d^{-2}f}{[d(x-a)]^{-2}} \\ &\quad + \frac{d^{-1}}{[d(x-a)]^{-1}}\left\{g^{(2)}\frac{d^{-2}f}{[d(x-a)]^{-2}}\right\}.\end{aligned} \tag{2.23}$$

Repeatedly applying this process indefinitely yields:

$$\begin{aligned}\frac{d^{-1}[fg]}{[d(x-a)]^{-1}} &= \sum_{j=0}^{\infty}\left[(-1)^j g^{(j)}\frac{d^{-1-j}f}{[d(x-a)]^{-1-j}}\right] \\ &= \sum_{j=0}^{\infty}\binom{-1}{j}g^{(j)}\frac{d^{-1-j}f}{[d(x-a)]^{-1-j}}.\end{aligned} \tag{2.24}$$

When (2.24) is integrated, using this same formula inside summation, and the composition rules for integrals and derivatives are applied, we obtain

$$\begin{aligned}
\frac{d^{-2}[fg]}{[d(x-a)]^{-2}} &= \sum_{j=0}^{\infty}\binom{-1}{j}\sum_{k=0}^{\infty}\binom{-1}{k}g^{(j+k)}\frac{d^{-j-k-2}f}{[d(x-a)]^{-j-k-2}} \\
&= \sum_{j=0}^{\infty}\sum_{l=j}^{\infty}\binom{-1}{j}\binom{-1}{l-j}g^{(l)}\frac{d^{-2-l}f}{[d(x-a)]^{-2-l}} \\
&= \sum_{l=0}^{\infty}\sum_{j=0}^{l}\binom{-1}{j}\binom{-1}{l-j}g^{(l)}\frac{d^{-2-l}f}{[d(x-a)]^{-2-l}} \\
&= \sum_{l=0}^{\infty}\binom{-2}{l}g^{(l)}\frac{d^{-2-l}f}{[d(x-a)]^{-2-l}}.
\end{aligned} \tag{2.25}$$

In the final steps of (2.25), we have made use of the permutation (2.95)

$$\sum_{k=0}^{\infty}\sum_{j=0}^{k} = \sum_{j=0}^{\infty}\sum_{k=j}^{\infty},$$

and the summation $\sum_{j=0}^{l}\binom{-1}{j}\binom{-1}{l-j} = \binom{-2}{l}$. The latter result is derived from the well-known summation formula (2.93)

$$\sum_{k=0}^{l}\binom{q}{k}\binom{Q}{l-k} = \binom{q+Q}{l},$$

the proof of which can be found in subsection 2.1.5. The proofs of all equalities and summations employed here are established in Section 3.1.3. Continuing the iteration of the procedure that yielded (2.25) from (2.24), we arrive at the desired formula:

$$\frac{d^{-n}[fg]}{[d(x-a)]^{-n}} = \sum_{j=0}^{\infty}\binom{-n}{j}g^{(j)}\frac{d^{-n-j}f}{[d(x-a)]^{-n-j}}, \tag{2.26}$$

with n being a positive integer greater or equal to 1. A general expression of the product rule for multiple differintegration combining (2.26) with the Leibniz's rule for repeated differentiation of a product is established in Section 2.1.4.

The Chain Rule for Multiple Derivatives

The chain rule for differentiation states that for two differentiable functions g and f defined in $\mathbb{R}$,

$$\frac{d}{dx}f(g(x)) = \frac{d}{du}f(u)\frac{d}{dx}g(x) = g'(x)f'(g(x)). \tag{2.27}$$

This formula, facilitating the differentiation of $g(u)$ with respect to x, given the derivatives of $g(u)$ with respect to u and u with respect to x, stands as one of the most crucial tools in integer differential calculus. However, the chain rule doesn't apply in fractional calculus due to the non-local nature of fractional derivatives, which incorporate information from the entire function rather than just a specific point or neighborhood. The proof for the chain rule from [2] heavily depends on the local nature of integer derivatives, as demonstrated below. Suppose f is differentiable at $u = g(a)$, g is differentiable at a, and $h(x) = f\left(g(x)\right)$. According to the definition of the derivative of h:

$$h'(a) = \lim_{x\to a} \frac{h(x) - h(a)}{x - a} = \lim_{x\to a} \frac{f\left(g(x)\right) - f\left(g(a)\right)}{x - a}. \tag{2.28}$$

We assume that $g(a) \neq g(x)$ for values of x near a but not equal to a.
We multiply the right hand of (2.28) by $\dfrac{g(x) - g(a)}{g(x) - g(a)}$, which equals 1, and let $v = g(x)$, and $u = g(a)$. This result is

$$\begin{aligned} h'(a) &= \lim_{x\to a} \frac{f\left(g(x)\right) - f\left(g(a)\right)}{g(x) - g(a)} \frac{g(x) - g(a)}{x - a} \\ &= \lim_{x\to a} \frac{f(v) - f(u)}{v - u} \frac{g(x) - g(a)}{x - a}. \end{aligned}$$

By assumption, g is differentiable at a; therefore it is continuous at a. This means that $\lim_{x\to a} g(x) = g(a)$, so $v \to u$ as $x \to a$. Consequently,

$$h'(a) = \lim_{v\to u} \frac{f(v) - f(u)}{v - u} \lim_{x\to a} \frac{g(x) - g(a)}{x - a} = f'(u)g'(a),$$

with $f'(u) = \lim\limits_{v\to u} \dfrac{f(v) - f(u)}{v - u}$ and $g'(a) = \lim_{x\to a} \dfrac{g(x) - g(a)}{x - a}$. Because f and g are differentiable at u and a, respectively, the two limits in this expression exist; therefore $h'(a)$ exists. Noting that $u = g(a)$, we have $h'(a) = f'\left(g(a)\right) g'(a)$. Replacing a with the variable x gives the chain rule $h'(x) = g'(x) f'\left(g(x)\right)$.

Iterated Integrals

Consider the formula

$$\frac{d^{-1} f}{\left[d(x-a)\right]^{-1}} = \int_a^x f(y)dy = \frac{1}{n!} \frac{d^n}{dx^n} \int_a^x \left[x - y\right]^n f(y)dy, \qquad n = 0, 1, 2, 3, \cdots \tag{2.29}$$

For $n = 0$, (2.29) is the identity (in this context the notational convention 0!=1 is used), while for $n = 1$, it follows easily from Leibniz's theorem for differentiation and integration. For general integer n, one need only notice that the evaluation of the integrand on the right-hand side at the upper limit x gives 0, while the differentiation n times inside the integral produces $n!f(y)$. A single integration of (2.29) for $n = 1$ produces:

$$\frac{d^{-2}f}{[d(x-a)]^{-2}} = \int_a^x \int_a^{x_1} f(x_0)\, dx_0\, dx_1 = \frac{1}{1!}\int_a^x [x-y]\, f(y)dy, \tag{2.30}$$

and an $(n-1)$-fold integration produces Cauchy's formula for repeated integration.

$$\frac{d^{-n}f}{[d(x-a)]^{-n}} = \int_a^x \int_a^{x_{n-1}} \cdots \int_a^{x_1} f(x_0)\, dx_0 \cdots dx_{n-1} = \frac{1}{(n-1)!}\int_a^x [x-y]^{n-1}\, f(y)dy. \tag{2.31}$$

Thus an iterated integral may be expressed as a weighted integral with a weight function, a fact that provides an important clue for generalizations involving non-integer orders.

Differentiation and Integration of Series

Many functions are often represented by infinite series expansions. Understanding the conditions for term-by-term differentiation or integration of such series is crucial. Below are two key results, with further extensions discussed in Section 2.1.4 for differintegrals of any order. Let $f_0, f_1, \ldots$ be functions defined and continuous on the interval $a \le x \le b$. Then,

$$\frac{d^{-1}}{[d(x-a)]^{-1}}\Big\{\sum_{j=0}^{\infty} f_j\Big\} = \sum_{j=0}^{\infty} \frac{d^{-1}f_j}{[d(x-a)]^{-1}}, \quad a \le x \le b, \tag{2.32}$$

assuming that the series $\sum f_j$ converges uniformly in the interval $a \le x \le b$. The conditions necessary to apply differentiation across the terms of an infinite series are slightly distinct. In this case, it is necessary for each f_j to possess continuous derivatives on $a \le x \le b$. Then,

$$\frac{d}{dx}\Big\{\sum_{j=0}^{\infty} f_j\Big\} = \sum_{j=0}^{\infty} \frac{df_j}{dx}, \quad a \le x \le b, \tag{2.33}$$

provided $\sum f_j$ converges pointwise and $\sum \dfrac{df_j}{dx}$ converges uniformly on the interval $a \le x \le b$. This demonstrates that a series of continuous functions, converging uniformly (thus defining a continuous function), can be integrated term by term. Similarly, a series of continuously differentiable functions, converging pointwisely, can be differentiated term by term, provided the resulting series of derivatives converges uniformly.

Differentiation and Integration of Powers

We gather here the elementary formulas that express $\dfrac{d^q[x-a]^p}{[d(x-a)]^q}$ for possible positive and negative integer values of q. We have

$$\frac{d^n[x-a]^p}{[d(x-a)]^n} = p[p-1]\cdots[p-n+1][x-a]^{p-n} = \frac{p![x-a]^{p-n}}{(p-n)!}, \quad n = 0, 1, \cdots \tag{2.34}$$

and

$$\frac{d^{-n}[x-a]^p}{[d(x-a)]^{-n}} = \int_a^x \int_a^{x_{n-1}} \cdots \int_a^{x_1} [x_0-a]^p dx_0 \cdots dx_{n-1} dx.$$
$$= \begin{cases} \dfrac{[x-a]^{p+n}}{[p+1][p+1]\cdots[p+n]}, & p > -1, \\ \\ \infty, & p \le -1, \quad n = 1, 2, \cdots \end{cases} \tag{2.35}$$

Let us highlight that for $p > -1$,

$$\frac{[x-a]^{p+n}}{[p+1][p+2]\cdots[p+n]} = \frac{[x-a]^{p+n}}{\dfrac{(p+n)!}{p!}} = \frac{p![x-a]^{p+n}}{(p+n)!} = \frac{p![x-a]^{p-(-n)}}{(p-(-n))!}.$$

Let us denote by q an integer of either sign and $p > -1$.
Upon substituting $q = n$, a positive integer, in equation (2.34), we obtain

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{p![x-a]^{p-q}}{(p-q)!} = \frac{\Gamma(p+1)[x-a]^{p-q}}{\Gamma(p-q+1)}. \tag{2.36}$$

Similarly, $q = -n$ in (2.35) leads to

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{\Gamma(p+1)[x-a]^{p-q}}{\Gamma(p-q+1)}. \tag{2.37}$$

Combining (2.36) and (2.37) yields

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \begin{cases} \infty, \quad q = -1, -2, \cdots, \quad p \le -1, \\ \\ \dfrac{\Gamma(p+1)[x-a]^{p-q}}{\Gamma(p-q+1)} \quad \begin{array}{ll} q = 0, 1, 2, \cdots, & \text{all } p \\ q = -1, -2, \cdots, & p > -1. \end{array} \end{cases} \tag{2.38}$$

The coefficient $\dfrac{\Gamma(p+1)}{\Gamma(p-q+1)}$ may be positive, negative or zero.

2.1.2 Fractional Derivatives and Integrals: Definitions and Equivalencies

Equation (2.13) defines an entity that we will refer to as a differintegral of an integer order. This can be extended to any real order q. In fact, nothing in the expression of (2.13) prevents it from being applied to real orders, and the Γ function present in its formula, which is an extension of the factorial to real numbers, smooths the whole process. In this chapter, we compare several definitions of the differintegral of a function f of an arbitrary order q. Perhaps the least ambiguous symbolism for the value at x of the differintegral of order q of a function defined on an interval $a \le y \le x$ would be

$$\frac{d^q f}{[d(y-a)]^q}, \quad q \in \mathbb{R}.$$

We shall eventually relate this differintegral to an ordinary integral in which y is a "dummy" variable of integration, and a and x are limits of integration. In line with conventions adopted in Section 2.1.1, our normal abbreviations for the q^{th} differintegral of the function f will be

$$\frac{d^q f}{[d(x-a)]^q}, \quad \text{and} \quad \frac{d^q f(x_0)}{[d(x-a)]^q} \quad \text{or} \quad \left[\frac{d^q f}{[d(x-a)]^q}\right]_{x=x_0}.$$

It being understood that f and $\dfrac{d^q f}{[d(x-a)]^q}$ are functions of the independent variable x when the x is omitted.

Differintegrable Functions

It is now time to define the class of functions to which we will apply differintegration operators. We will primarily focus on classically defined functions. For such classically defined functions, we follow the principles of integral calculus and stipulate that our candidate functions must be defined on the closed interval $a \leq y \leq x$, bounded everywhere in the half-open interval $a < y \leq x$, and be "well behaved" at the lower limit a (i.e not diverge at the lower limit a). Good examples of such functions are polynomials, exponential, logarithms and all functions whose differintegrals can be determined. In this section, we will direct our attention to a category known as "differintegrable series", defined as finite sums of functions, each of which can be expressed as

$$f(y) = [y-a]^p \sum_{j=0}^{\infty} c_j [y-a]^{\frac{j}{n}}, \quad c_0 \neq 0, \quad p > -1, \quad n \geq 1, \text{ an integer.} \tag{2.39}$$

Notice that p has been chosen to ensure that the leading coefficient is nonzero. Such differintegrable series f then satisfy

$$\lim_{y \to a} \Big\{ [y-a] f(y) \Big\} = 0.$$

An important consequence of this representation is that given the fact that

$$\begin{aligned} \sum_{j=0}^{\infty} \frac{j}{n} = 0 + \frac{1}{n} + \frac{2}{n} + \cdots + \frac{n-1}{n} + & \\ 1 + \left(1 + \frac{1}{n}\right) + \left(1 + \frac{2}{n}\right) + \cdots \left(1 + \frac{n-1}{n}\right) + & \\ 2 + \left(2 + \frac{1}{n}\right) + \left(2 + \frac{2}{n}\right) + \cdots \left(2 + \frac{n-1}{n}\right) + & \\ N + \left(N + \frac{1}{n}\right) + \left(N + \frac{2}{n}\right) + \cdots \left(N + \frac{n-1}{n}\right) + \cdots & \end{aligned}$$

Let us consider the following result:

$$\begin{aligned}\sum_{j=0}^{\infty}\frac{j}{n} &= 0+1+2+3+4+\cdots+N+\cdots\\ &\quad+\frac{1}{n}+\left(1+\frac{1}{n}\right)+\left(2+\frac{1}{n}\right)+\cdots+\left(N+\frac{1}{n}\right)+\cdots\\ &\quad+\frac{2}{n}+\left(1+\frac{2}{n}\right)+\left(2+\frac{2}{n}\right)+\cdots+\left(N+\frac{2}{n}\right)+\cdots\\ &\quad+\frac{n-1}{n}+\left(1+\frac{n-1}{n}\right)+\left(2+\frac{n-1}{n}\right)+\cdots+\left(N+\frac{n-1}{n}\right)+\cdots\end{aligned}$$

Let us denote

$$\begin{aligned}&\sum_{j_1=0}^{\infty} j_1 = 0+1+2+3+4+\cdots+N+\cdots\\ &\sum_{j_2=0}^{\infty}\left(j_2+\frac{1}{n}\right) = \frac{1}{n}+\left(1+\frac{1}{n}\right)+\left(2+\frac{1}{n}\right)+\cdots+\left(N+\frac{1}{n}\right)+\cdots\\ &\sum_{j_n=0}^{\infty}\left(j_n+\frac{n-1}{n}\right) = \frac{n-1}{n}+\left(1+\frac{n-1}{n}\right)+\left(2+\frac{n-1}{n}\right)+\cdots+\left(N+\frac{n-1}{n}\right)+\cdots.\end{aligned}$$

We then finally have

$$\sum_{j=0}^{\infty}\frac{j}{n}=\sum_{j_1=0}^{\infty}j_1+\sum_{j_2=0}^{\infty}\left(j_2+\frac{1}{n}\right)+\cdots+\sum_{j_n=0}^{\infty}\left(j_n+\frac{n-1}{n}\right).$$

Utilizing this result in (2.39) leads to the following decomposition of f as a finite sum of units of power series.

$$f(y)=[y-a]^p\sum_{j_1=0}^{\infty}c_{j_1}[y-a]^{j_1}+[y-a]^{[np+1]/n}\sum_{j_2=0}^{\infty}c_{j_2}[y-a]^{j_2}+\cdots+[y-a]^{[np+n-1]/n}\sum_{j_n=0}^{\infty}c_{j_n}[y-a]^{j_n},$$

of n differintegrable units f_v, each of which is a product of a power(greater than -1) of $(y-a)$ and a function analytic in $(y-a)$. The desirability of this property will become more apparent in the subsequent sections.

Fundamental Definitions

The initial definition we present is what we consider the most fundamental, because it imposes the fewest restrictions on the functions it applies to and avoids explicit use of the concepts of ordinary derivative and integral. This definition, which directly extends and unifies notions of difference quotients and Riemann sums, was first introduced by Grünwald (1867) and later expanded by Post (1930). Referring to Section 2.1.1 and the discussion leading to equation (2.13), we define the differintegral of order q using the formula:

$$\frac{d^q f(x)}{[d(x-a)^q]} = \lim_{\delta x \to 0} \left\{ \frac{[\delta x]^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x - j\ \delta x) \right\}, \tag{2.40}$$

where q is arbitrary.

Note:

On one hand, if $q < 0$, $N \geq 1$ represents the number of subdivisions employed in defining an integral as a limit of sums. On the other hand, if $q \geq 0$, in order to unify the formula of the n^{th} derivative with one that defines an integral as a limit of sums, we define the derivatives in terms of a restricted limit. This limit occurs as δx tends to zero through discrete values only, by setting $\delta x = \dfrac{[x-a]}{N}, \quad N = 1, 2, \cdots.$

It is worth noting that this definition solely relies on evaluations of the function itself; no explicit use is made of derivatives or integrals of f. However, the most commonly encountered definition of an integral of fractional order is through an integral operator known as the Riemann-Liouville integral. To justify this definition, one only needs to consider Cauchy's formula in equation (2.31) and replace "$-n$" with q, suggesting the generalization to non-integer orders:

$$\left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L} = \frac{1}{\Gamma(-q)} \int_a^x [x-y]^{-q-1} f(y) dy, \quad q < 0. \tag{2.41}$$

In equation (2.41), we have utilized the subscript $[\cdots]_{R-L}$ to denote the Riemann-Liouville fractional integral, which may be distinct from our more fundamental definition in (2.40). We will now demonstrate that the two definitions produce identical outcomes, and the subscript $[\cdots]_{R-L}$ will be omitted thereafter. Formula (2.41) will be retained as the $q < 0$ definition of the differintegral; it is extended to $q \geq 0$ by insisting that equation (2.41) satisfies by the "restricted composition".

$$\left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L} = \frac{d^n}{dx^n} \left[\frac{d^{q-n} f}{[d(x-a)]^{q-n}}\right]_{R-L}, \tag{2.42}$$

where $\dfrac{d^n}{dx^n}$ denotes ordinary n-fold differentiation and n is an integer chosen large enough so that $q - n < 0$. Together with equation (2.41), definition (2.42) then defines the operator

$$\left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L}, \tag{2.43}$$

for all q. Before demonstrating the equivalence between the two differintegral formulas (2.40) and (2.43), it is necessary to establish the "restricted composition rule" for (2.40). This rule is utilized for both (2.40) and (2.41) in the proof of equivalence.
Based on definition (2.40), we aim to demonstrate that

$$\frac{d^n}{dx^n}\left[\frac{d^q f}{[d(x-a)]^q}\right] = \frac{d^{n+q} f}{[d(x-a)]^{n+q}}, \tag{2.44}$$

for all positive integers n and all q. One might consider this property as a limited composition law, i.e., a rule for composing orders of the generalized differintegral. To validate this assertion, let $\delta x = \dfrac{x-a}{N}$,

$$\frac{d^q f(x)}{[d(x-a)]^q} = \lim_{\delta x\to 0}\left\{\frac{[\delta x]^{-q}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)} f(x-j\ \delta x)\right\}.$$

Upon subdividing the interval $a \le y \le x - \delta x$ into only $N-1$ equally spaced subintervals, we see that

$$\begin{aligned}\frac{d^q f}{[d(x-a)]^q}(x-\delta x) &= \lim_{\delta x\to 0}\left\{\frac{[\delta x]^{-q}}{\Gamma(-q)}\sum_{j=0}^{N-2}\frac{\Gamma(j-q)}{\Gamma(j+1)} f(x-\delta x-j\ \delta x)\right\}\\ &= \lim_{\delta x\to 0}\left\{\frac{[\delta x]^{-q}}{\Gamma(-q)}\sum_{j=1}^{N-1}\frac{\Gamma(j-q-1)}{\Gamma(j)} f(x-j\ \delta x)\right\}.\end{aligned}$$

On differentiation making use of restricted limits as explained at the start of section (2.1) to define $\dfrac{d}{dx}$, one gets

$$\begin{aligned}\frac{d}{dx}\left[\frac{d^q f}{[d(x-a)]^q}\right] &= \lim_{N\to\infty}\left\{[\delta x]^{-1}\left[\frac{d^q f}{[d(x-a)]^q}(x) - \frac{d^q f}{[d(x-a)]^q}(x-\delta x)\right]\right\}\\ &= \lim_{N\to\infty}\left\{\frac{[\delta x]^{-q-1}}{\Gamma(-q)}\left[\Gamma(-q) f(x) + \sum_{j=1}^{N-1}\left\{\frac{\Gamma(j-q)}{\Gamma(j+1)} - \frac{\Gamma(j-q-1)}{\Gamma(j)}\right\}\right]\right\}.\end{aligned}$$

Making use of the recurrence properties of the Γ function,

$$\frac{\Gamma(j-q)}{\Gamma(j+1)} - \frac{\Gamma(j-q-1)}{\Gamma(j)} = \frac{\Gamma(-q)\Gamma(j-q-1)}{\Gamma(-q-1)\Gamma(j+1)},$$

is obtained. Therefore,

$$\begin{aligned}\frac{d}{dx}\left[\frac{d^q f}{[d(x-a)]^q}\right] &= \lim_{N\to\infty}\left\{\frac{[\delta x]^{-q-1}}{\Gamma(-q-1)}\left[\sum_{j=0}^{N-1}\frac{\Gamma(j-q-1)}{\Gamma(j+1)} f(x-j\ \delta x)\right]\right\}\\ &= \frac{d^{q+1}}{[d(x-a)]^{q+1}}.\end{aligned}$$

Equation (2.44) follows by induction.

Equivalence of Definitions

It is now relevant to inquire whether the Riemann-Liouville definition, based on equation (2.41) for negative q and its extension to $q \geq 0$ by means of equation (2.42), yields operators that coincide for all functions f. We will demonstrate that this is indeed the case. Firstly, we establish the identity for a subset of q values and then utilize property (2.42) to extend the identity to all orders q. To begin, let f be an arbitrary but fixed function on the interval $a \leq y \leq x$. As before, we define $\delta x = \dfrac{x-a}{N}$, then the difference

$$\begin{aligned}
\Delta &= \frac{d^q f}{[d(x-a)]^q}(x) - \left[\frac{d^q f}{[d(x-a)]^q}(x)\right]_{R-L} \\
&= \lim_{\delta x \to 0}\left\{\frac{[\delta x]^{-q}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)}f(x-j\ \delta x)\right\} - \int_0^{x-a}\frac{f(x-u)}{\Gamma(-q)u^{1+q}}du \\
&= \lim_{\delta x \to 0}\left\{\frac{[\delta x]^{-q}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)}f(x-j\ \delta x)\right\} - \lim_{\delta x \to 0}\sum_{j=0}^{N-1}\frac{f(x-j\ \delta x)\delta x}{\Gamma(-q)[j\ \delta x]^{1+q}} \\
&= \lim_{N \to \infty}\left\{\frac{[\delta x]^{-q}}{\Gamma(-q)}\sum_{j=0}^{N-1}f(x-j\ \delta x)\left[\frac{\Gamma(j-q)}{\Gamma(j+q)} - j^{-1-q}\right]\right\} \\
&= \frac{[x-a]^{-q}}{\Gamma(-q)}\lim_{N \to \infty}\left\{\sum_{j=0}^{N-1}f\Big(\frac{Nx-jx+ja}{N}\Big)N^q\left[\frac{\Gamma(j-q)}{\Gamma(j+q)} - j^{-1-q}\right]\right\}.
\end{aligned} \tag{2.45}$$

The N terms within the summation are divided into two groups: $0 \leq j \leq J-1$ and $J \leq j \leq N-1$, where J is independent of N. Thus

$$\begin{aligned}
\Delta = &\frac{[x-a]^{-q}}{\Gamma(-q)}\lim_{N \to \infty}\left\{\sum_{j=0}^{J-1}f\Big(\frac{Nx-jx+ja}{N}\Big)N^q\left[\frac{\Gamma(j-q)}{\Gamma(j+q)} - j^{-1-q}\right]\right\} \\
&+ \frac{[x-a]^{-q}}{\Gamma(-q)}\lim_{N \to \infty}\left\{\frac{1}{N}\sum_{j=J}^{N-1}f\Big(\frac{Nx-jx+ja}{N}\Big)\left[\frac{j}{N}\right]^{-2-q}\right]\left[\frac{q[q+1]}{2N} + \frac{\mathcal{O}(j^{-1})}{N}\right]\right\},
\end{aligned} \tag{2.46}$$

where N is sufficiently large to validate the asymptotic expansion for terms in the second group. Now, for $q < -1$, the J bracketed terms within the first summation are bounded. Hence, if $f\Big(\dfrac{Nx-jx+ja}{N}\Big)$ is also bounded for j within the first group, the presence of the N^q factor ensures that the first sum vanishes in the limit $N \to \infty$. Examining the three factors within the second summation, we note that $\left[\dfrac{j}{N}\right]^{-2-q}$ is always less than unity if $q \leq -2$, and that the third factor tends to zero as $N \to \infty$. Therefore, if $f\Big(\dfrac{Nx-jx+ja}{N}\Big)$ is bounded for

j within the second group, each term in the second summation vanishes since $\frac{1}{N} \to 0$ when $N \to \infty$. The above demonstrates that if f is bounded on $a < y \leq x$ and if $q \leq -2$, then

$$\Delta = \frac{d^q f}{[d(x-a)]^q}(x) - \left[\frac{d^q f}{[d(x-a)]^q}(x)\right]_{R-L} \equiv 0, \tag{2.47}$$

Thus, the two definitions, when applied to functions bounded in this manner, are indeed identical for $q \leq -2$. This fact, along with property (2.42) and requirement (2.44) , demonstrates that the two definitions are identical for any q. Indeed, for arbitrary q, we know that for any positive integer n

$$\left[\frac{d^q f}{[d(x-a)]^q}\right] = \frac{d^n}{dx^n}\left\{\frac{d^{q-n} f}{[d(x-a)]^{q-n}}\right\}$$

and

$$\left[\frac{d^q f}{[d(x-a)]^q}\right]_{R-L} = \frac{d^n}{dx^n}\left\{\frac{d^{q-n} f}{[d(x-a)]^{q-n}}\right\}.$$

One need only choose n sufficiently large that $q - n \leq -2$ and make use of (2.47) to complete the proof.

Fractional Calculus for Complex Numbers

A different avenue for motivating the definition of the differintegral stems from consideration of Cauchy's integral formula. The Cauchy's integral formula is a powerful result in complex analysis which provides a method for computing higher order derivatives of a complex valued function within a simply connected domain using contour integration.

The formula states that if $f(z)$ is an analytic function within a simply connected domain D containing a closed contour C, and z is a point inside C, then the nth derivative of $f(z)$ at z is given by:

$$\frac{d^n f(z)}{dz^n} = \frac{n!}{2\pi i}\oint_C \frac{f(\xi)}{[\xi - z]^{n+1}} d\xi,$$

where:

- $\oint_C$ denotes the counter-clockwise integral along the closed contour C. Contour integrals involve integrating a complex valued function along a path in the complex plane, known as a contour. Contour refers to a curve or a path in the complex plane. These curves are typically defined by parametric equations or by specifying points along the curve.
- $f(\xi)$ represents the value of the function $f(z)$ at point ξ on the contour C.
- i denotes the imaginary unit and is defined as $i = \sqrt{-1}$.

- A region D in the complex plane is said to be simply connected if any two points in D can be joined by a path lying entirely within D, and if every simple closed curve in D can be continuously shrunk to a point without leaving D.

When the positive integer n is replaced by a non-integer q, the expression $[\xi - z]^{-q-1}$ no longer has a pole at $\xi = z$ but a branch point. In this case, one cannot freely deform the contour C surrounding z since the integral will depend on the location of the point at which C crosses the branch line for $[\xi - z]^{-q-1}$. A branch line is a line in the complex plane across which a complex-valued function undergoes a discontinuity or a change in behavior. The point is chosen to be 0 and the branch line to be the straight line joining 0 and z, in the quadrant $\Re(\xi) \leq 0$, $\Im(\xi) \leq 0$ as shown in Figure 2.1. Then, for q not a negative integer, one simply defines:

$$\frac{d^q f(z)}{dz^q} = \frac{\Gamma(q+1)}{2\pi i} \oint_C \frac{f(\xi)}{[\xi - z]^{q+1}} d\xi, \tag{2.48}$$

where the contour C begins and ends at $\xi = 0$ enclosing z once in a contour traversed counter-clockwise. To uniquely specify the denominator of the integrand, one defines

$$[\xi - z]^{q+1} = \exp\left([q+1] \log(\xi - z)\right),$$

where $\log(\xi - z)$ is real if ξ and z are both real numbers and $\xi > z$. We can relate definition (2.48) to that of Riemann-Liouville by first deforming the contour C into a contour C' lying on both sides of the branch line. One finds that

$$\frac{\Gamma(q+1)}{2\pi i} \oint_{C'} \frac{f(\xi)}{[\xi - z]^{q+1}} d\xi = \frac{\Gamma(q+1)}{2\pi i} \left\{ \int_{C_1} \frac{f(\xi)}{[\xi - z]^{q+1}} d\xi + \int_{C_2} \frac{f(\xi)}{[\xi - z]^{q+1}} d\xi + \int_{C_3} \frac{f(\xi)}{[\xi - z]^{q+1}} d\xi \right\}, \tag{2.49}$$

where C_1 denotes the segment below the branch line and joining the point 0 to a close neighborhood of z, C_2 the circular contour around z and C_3 the segment above the branch line and joining a close neighborhood of z to the point 0 as shown in Figure 2.1.

Parameterization:

- $C_1 : \xi = \mu - i\epsilon, \quad 0 \leq \mu \leq z, \quad \epsilon \to 0^+,$
- $C_2 : \xi - z = r \exp(i\theta), \quad -\pi \leq \theta \leq \pi,$ and $r \to 0^+,$
- $C_3 : \xi = z - \mu + i\epsilon, \quad 0 \leq \mu \leq z \quad \epsilon \to 0^+.$

Thus,

$$I_1 = \lim_{\epsilon \to 0^+} \int_{C_1} \frac{f(\xi)}{[\xi - z]^{q+1}} d\xi = \lim_{\epsilon \to 0^+} \int_0^z \frac{f(\mu - i\epsilon)}{[\mu - i\epsilon - z]^{q+1}} d\mu.$$

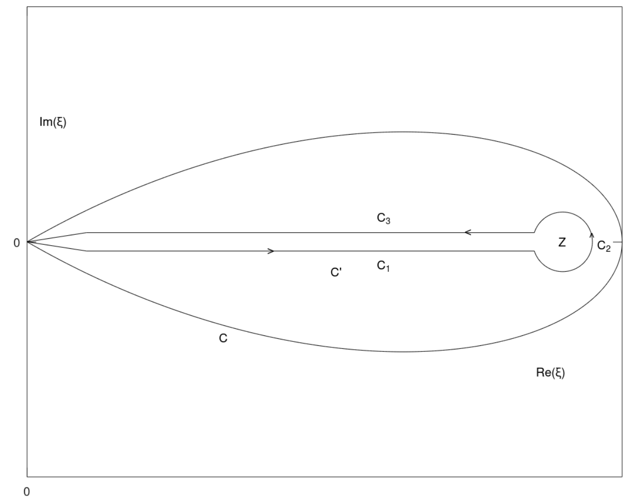


Figure 2.1: The Cauchy contour C is deformed into C' for the purpose of implementing the Cauchy's integral formula.

Subsequently,

$$\int_{C_2} \frac{f(\xi)}{[\xi - z]^{q+1}} d\xi = \int_{-\pi}^{\pi} \frac{f(z + r\exp(i\theta))}{[r\exp(i\theta)]^{q+1}} ri\exp(i\theta) d\theta.$$

We have

$$\begin{aligned}\left| \int_{-\pi}^{\pi} \frac{f(z + r\exp(i\theta))}{[r\exp(i\theta)]^{q+1}} ri\exp(i\theta) d\theta \right| &\leq \int_{-\pi}^{\pi} \left| \frac{f(z + r\exp(i\theta))}{[r\exp(i\theta)]^{q+1}} ri\exp(i\theta) \right| d\theta \\ &= \int_{-\pi}^{\pi} \frac{\left| f(z + r\exp(i\theta)) \right|}{[r\exp(i\theta)]^{q+1}} \left| ri\exp(i\theta) \right| d\theta \\ &= \int_{-\pi}^{\pi} \frac{\left| f(z + r\exp(i\theta)) \right|}{|r|^{q+1}} |r| d\theta.\end{aligned}$$

Since $q < 0$,

$$\lim_{r\to 0^+} \frac{\left| f(z + r\exp(i\theta)) \right|}{|r|^{q+1}} |r| = 0 \Rightarrow \lim_{r\to 0^+} \int_{-\pi}^{\pi} \frac{f(z + r\exp(i\theta))}{[r\exp(i\theta)]^{q+1}} ri\exp(i\theta) d\theta = 0.$$

Then, for $r \to 0^+$,

$$\int_{C_2} \frac{f(\xi)}{[\xi - z]^{q+1}} d\xi \to 0.$$

Moreover,

$$I_3 = \int_{C_3} \frac{f(\xi)}{[\xi - z]^{q+1}} d\xi = \int_0^z \frac{f(z-\mu+i\epsilon)}{[z-\mu+i\epsilon-z]^{q+1}}(-d\mu) = -\int_0^z \frac{f(z-\mu+i\epsilon)}{[-\mu+i\epsilon]^{q+1}} d\mu.$$

Upon setting $\zeta = z - \mu$, this leads to

$$I_3 = -\lim_{\epsilon \to 0} \int_0^z \frac{f(\zeta + i\epsilon)}{[\zeta - z + i\epsilon]^{q+1}} d\zeta. \tag{2.50}$$

Let us compare I_1 andI_3. Since I_1 and I_3 have the same integration boundaries, we just have to compare their integrands. Additionally, their integrands are both complex functions; comparing them is equivalent to comparing their modulis and arguments. Let

$$A_1 = \frac{f(\mu - i\epsilon)}{[\mu - i\epsilon - z]^{q+1}} \Rightarrow |A_1| = \left| \frac{f(\mu - i\epsilon)}{[\mu - i\epsilon - z]^{q+1}} \right|.$$

Knowing that

$$[\mu - i\epsilon - z]^{q+1} = \exp\Big([q+1]\log(\mu - i\epsilon - z)\Big),$$

with $\log(\mu - i\epsilon - z) = \ln|\mu - i\epsilon - z| + i\,\mathrm{Arg}\,(\mu - i\epsilon - z)$, and $Arg(\theta)$ being the argument of θ on the principal branch. We finally have

$$[\mu - i\epsilon - z]^{q+1} = \exp\Big([q+1]\ln|\mu - i\epsilon - z|\Big)\exp\Big(i[q+1]\,\mathrm{Arg}\,(\mu - i\epsilon - z)\Big).$$

This leads to

$$\begin{aligned}
\arg(A_1) &= \arg\left(\frac{f(\mu - i\epsilon)}{[\mu - i\epsilon - z]^{q+1}}\right) \\
&= \arg\Big(f(\mu - i\epsilon)\Big) - \arg\Big([\mu - i\epsilon - z]^{q+1}\Big) \\
&= \arg\Big(f(\mu - i\epsilon)\Big) - \arg\left(\exp\Big([q+1]\ln|\mu - i\epsilon - z|\Big)\exp\Big(i[q+1]\,\mathrm{Arg}\,(\mu - i\epsilon - z)\Big)\right) \\
&= \arg\Big(f(\mu - i\epsilon)\Big) - [q+1]\,\mathrm{Arg}\Big(\mu - i\epsilon - z\Big).
\end{aligned}$$

For $\mu = \zeta$, we finally have

$$|A_1| = \left| \frac{f(\zeta - i\epsilon)}{[\zeta - i\epsilon - z]^{q+1}} \right|,$$

and

$$\arg(A_1) = \arg\Big(f(\zeta - i\epsilon)\Big) - [q+1]\,\mathrm{Arg}\Big(\zeta - i\epsilon - z\Big).$$

Similarly,

$$|A_3| = \left|\frac{f(\zeta+i\epsilon)}{[\zeta+i\epsilon-z]^{q+1}}\right|,$$

and

$$\arg(A_3) = \arg\Big(f(\zeta+i\epsilon)\Big) - [q+1]\,\mathrm{Arg}\Big(\zeta+i\epsilon-z\Big).$$

Going from $\zeta-i\epsilon-z$ to $\zeta+i\epsilon-z$ requires a rotation of 2π, then

$$\mathrm{Arg}\Big(\zeta+i\epsilon-z\Big) = \mathrm{Arg}\Big(\zeta-i\epsilon-z\Big) + 2\pi.$$

This leads to

$$\arg(A_3) = \arg\Big(f(\zeta+i\epsilon)\Big) - [q+1]\Big(\mathrm{Arg}\Big(\zeta-i\epsilon-z\Big)+2\pi\Big).$$

When $\epsilon \to 0^+$, we finally have

$$\begin{aligned} |A_1| = |A_3| \quad \text{and} \quad \arg(A_3) = \arg(A_1) - 2\pi[q+1] \Rightarrow &\quad A_3 = A_1 \exp\Big(-2\pi i[q+1]\Big) \\ \Rightarrow &\quad I_3 = I_1 \exp\Big(-2\pi i[q+1]\Big). \end{aligned}$$

We finally obtain for $\zeta = \xi$

$$\begin{aligned} \oint_{C'} \frac{f(\xi)}{[\xi-z]^{q+1}}d\xi &= \int_0^z \frac{f(\xi)}{[\xi-z]^{q+1}}d\xi - \exp\left(-2\pi i[q+1]\right)\int_0^z \frac{f(\xi)}{[\xi-z]^{q+1}}d\xi \\ &= \Big(1-\exp\left(-2\pi i[q+1]\right)\Big)\int_0^z \frac{f(\xi)}{[\xi-z]^{q+1}}d\xi. \end{aligned}$$

Substituting this result in (2.44) leads to

$$\frac{\Gamma(q+1)}{2\pi i}\oint_{C'} \frac{f(\xi)}{[\xi-z]^{q+1}}d\xi = \frac{\Gamma(q+1)}{2\pi i}\Big(1-\exp\left(-2\pi i[q+1]\right)\Big)\int_0^z \frac{f(\xi)}{[\xi-z]^{q+1}}d\xi.$$

Let us compute $\dfrac{\Gamma(q+1)}{2\pi i}\Big(1-\exp\left(-2\pi i[q+1]\right)\Big)$:
On one hand,

$$\begin{aligned} 1-\exp\left(-2\pi i[q+1]\right) &= 1 - \Big\{\cos\left(2\pi[q+1]\right) - i\sin\left(2\pi[q+1]\right)\Big\} \\ &= 1-\cos\left(2\pi[q+1]\right) + i\sin\left(2\pi[q+1]\right). \end{aligned} \tag{2.51}$$

On the other hand, using the reflection property of the Γ function, we have

$$\frac{\Gamma(q+1)}{2\pi i} = \frac{\pi}{2\pi i\sin\Big(\pi(q+1)\Big)\Gamma(-q)} = \frac{1}{2i\sin\Big(\pi(q+1)\Big)\Gamma(-q)}. \tag{2.52}$$

Combining (2.51) and (2.52) gives

$$
\begin{aligned}
\frac{\Gamma(q+1)}{2\pi i}\Big(1-\exp\left(-2\pi i[q+1]\right)\Big) &= \frac{1-\cos\left(2\pi[q+1]\right)+i\sin\left(2\pi[q+1]\right)}{2i\sin\Big(\pi(q+1)\Big)\Gamma(-q)} \\
&= \frac{2\sin^2\Big(\pi(q+1)\Big)+2i\cos\Big(\pi(q+1)\Big)\sin\Big(\pi(q+1)\Big)}{2i\sin\Big(\pi(q+1)\Big)\Gamma(-q)} \\
&= \frac{\sin\Big(\pi(q+1)\Big)+i\cos\Big(\pi(q+1)\Big)}{i\Gamma(-q)} \\
&= \frac{-i\sin\Big(\pi(q+1)\Big)+\cos\Big(\pi(q+1)\Big)}{\Gamma(-q)} \\
&= \frac{\exp\left(-\pi i[q+1]\right)}{\Gamma(-q)}.
\end{aligned}
$$

Then,

$$
\begin{aligned}
\oint_{C'}\frac{f(\xi)}{[\xi-z]^{q+1}}d\xi &= \frac{\Gamma(q+1)}{2\pi i}\Big(1-\exp\left(-2\pi i[q+1]\right)\Big)\int_0^z\frac{f(\xi)}{[\xi-z]^{q+1}}d\xi \\
&= \frac{\exp\left(-\pi i[q+1]\right)}{\Gamma(-q)}\int_0^z\frac{f(\xi)}{[\xi-z]^{q+1}}d\xi \\
&= \frac{1}{\Gamma(-q)}\int_0^z\frac{f(\xi)}{\exp\left(\pi i[q+1]\right)[\xi-z]^{q+1}}d\xi \\
&= \frac{1}{\Gamma(-q)}\int_0^z\frac{f(\xi)}{\Big[\exp\left(\pi i\right)[\xi-z]\Big]^{q+1}}d\xi \\
&= \frac{1}{\Gamma(-q)}\int_0^z\frac{f(\xi)}{\Big[(-1)\cdot[\xi-z]\Big]^{q+1}}d\xi \\
&= \frac{1}{\Gamma(-q)}\int_0^z\frac{f(\xi)}{[z-\xi]^{q+1}}d\xi.
\end{aligned}
$$

This is the Riemann-Liouville definition with $a=0$. Definition (2.48) is attributed by Oster (1970a) to Nekrassov (1808). Erdélyi (1964) defined a q-th-order differintegral of a function $f(z)$ with respect to the function z^n by:

$$
\frac{d^q f(z)}{[d(z^n-a^n)]^q} = \frac{1}{\Gamma(-q)}\int_a^z\frac{f(\xi)n\xi^{n-1}}{[z^n-\xi^n]^{q+1}}d\xi.
$$

The types of derivatives reviewed above are considered classical fractional derivatives, since they were posed shortly after the integer calculus became widely accepted. In the 20^{th} century numerous other types of derivatives were defined and some of the properties discussed above were lost in favour of other more important ones. This will be discussed further in the following section.

Other Formulas Applicable To Analytic Functions

The aim of this section is to explore alternative representations for $\frac{d^q}{[d(x-a)]^q}$ concerning real analytic functions. These functions, denoted as ϕ, possess convergent power series expansions within the interval $a \leq y \leq x$. Such representations introduce computational flexibility for evaluating q-th order differintegrals for specific ϕ choices. Initially, our focus is on $q < 0$, allowing us to utilize the Riemann-Liouville definition. Thus,

$$\frac{d^q\phi}{[d(x-a)]^q} = \frac{1}{\Gamma(-q)}\int_a^x \frac{\phi(y)}{(x-y)^{q+1}}dy = \frac{1}{\Gamma(-q)}\int_0^{x-a} \frac{\phi(x-v)}{v^{q+1}}dv, \tag{2.53}$$

with $v = x - y$. Upon Taylor expansion of $\phi(x-v)$ about x, one has

$$\phi(x-v) = \phi - v\phi^{(1)} + \frac{v^2}{2!}\phi^{(2)} - \cdots = \sum_{k=0}^{\infty} \frac{(-v)^k \phi^{(k)}}{k!}. \tag{2.54}$$

The representation (2.54) involves no remainder since we have assumed that ϕ possesses a convergent power series expansion, and since such an expansion is unique. When this expansion is inserted into (2.53) and term-by-term integration is performed, the result is

$$\frac{d^q\phi}{[d(x-a)]^q} = \sum_{k=0}^{\infty} \frac{(-1)^k (x-a)^{k-q}\phi^{(k)}}{\Gamma(-q)(k-q)k!}. \tag{2.55}$$

2.1.3 Differentiation of Simple Functions

The purpose of this chapter is to calculate the q^{th} order differintegral of certain simple functions. The simple functions considered are examples of power functions $[x-a]^p$. Thus, we first examine the instances where $p = 0$ and $p = 1$, with the general case being explored just after.

The Zero Function

When definition (2.13) is applied to the function defined by $f \equiv c$, c any constant including zero, we see that

$$\begin{aligned} \frac{d^q[c]}{[d(x-a)]^q} = c\frac{d^q[1]}{[d(x-a)]^q} &= c \lim_{N\to\infty}\left\{\left[\frac{N}{x-a}\right]^q \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)}\right\} \\ &= c\frac{[x-a]^{-q}}{\Gamma(1-q)}. \end{aligned} \tag{2.56}$$

The final expression is obtained upon applying first (2.91):

$$\sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)} = \frac{\Gamma(N-q)}{\Gamma(1-q)\Gamma(N)},$$

and (2.87):

$$\lim_{j\to\infty}\left[j^{c+q}\frac{\Gamma(j-q)}{\Gamma(j)}\right]=\begin{cases}\infty, & c>0,\\ 1, & c=0,\\ 0, & c<0,\end{cases}$$

the proof of which can be found in subsection 2.1.5. Since $\dfrac{d^q[1]}{[d(x-a)]^q}$ is never infinite for $x>a$, we conclude by setting $c=0$ that

$$\frac{d^q[0]}{[d(x-a)]^q}=0, \quad \text{for all} \quad q. \tag{2.57}$$

Result (2.56) may appear obvious. However, as an example of its importance, observe that it provides a powerful counterexample to the thesis that if

$$\frac{d^q f}{[d(x-a)]^q}=g, \quad \text{then} \quad \frac{d^{-q}g}{[d(x-a)]^{-q}}=f,$$

for if f yields zero upon differentiation to order q, f cannot be restored by q-order integration. Here again, we encounter the so called composition rule, this time for non-integer orders. This subject will be more thoroughly explored in section 2.1.4.

The Unit Function

We consider the differintegral to order q of the function $f\equiv 1$. A straightforward application of (2.40) to the function $f\equiv 1$ gives

$$\frac{d^q[1]}{[d(x-a)]^q}=\lim_{N\to\infty}\left\{\left[\frac{N}{x-a}\right]^q\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)}\right\}.$$

Application first of (2.91) and (2.87) as for the zero function yields

$$\frac{d^q[1]}{[d(x-a)]^q}=\lim_{N\to\infty}\left\{\left[\frac{N}{x-a}\right]^q\frac{\Gamma(N-q)}{\Gamma(1-q)\Gamma(N)}\right\}=\frac{[x-a]^{-q}}{\Gamma(1-q)}, \tag{2.58}$$

as a result. As an example of the application of the unit function and its differintegrals, consider the combination of formulas (2.55) and (2.58) into

$$\frac{d^q\phi}{[d(x-a)]^q}=\sum_{k=0}^{\infty}[-1]^k\frac{\Gamma(1+k-q)}{\Gamma(-q)[k-q]k!}\frac{d^{q-k}[1]}{[d(x-a)]^{q-k}}\phi^{(k)}, \tag{2.59}$$

valid for any analytic function ϕ. Application of the recurrence property of the Gamma function as well as (2.89), the proof of which can be found in subsection 2.1.5 leads to the concise representation

$$\frac{d^q\phi}{[d(x-a)]^q} = \sum_{k=0}^{\infty} \binom{q}{k} \frac{d^{q-k}[1]}{[d(x-a)]^{q-k}} \frac{d^k\phi}{[d(x-a)]^k}, \tag{2.60}$$

where

$$\binom{q}{k} = \frac{\Gamma(q+1)}{k!\Gamma(q-k+1)}.$$

The function $x - a$

For the function $f(x) = x - a$, definition (2.40) gives

$$\begin{aligned}
\frac{d^q[x-a]}{[d(x-a)]^q} &= \lim_{N\to\infty} \left\{ \left[\frac{N}{x-a}\right]^q \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)} \left[\frac{Nx - jx + ja}{N} - a\right] \right\} \\
&= [x-a]^{1-q} \left[\lim_{N\to\infty} \left\{ N^q \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)} \right\} - \lim_{N\to\infty} \left\{ N^{q-1} \sum_{j=0}^{N-1} j \frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)} \right\} \right] \\
&= [x-a]^{1-q} \left[\lim_{N\to\infty} N^q \frac{\Gamma(N-q)}{\Gamma(1-q)\Gamma(N)} - \lim_{N\to\infty} N^{q-1} \left\{ \frac{-q\Gamma(N-q)}{\Gamma(2-q)\Gamma(N-1)} \right\} \right].
\end{aligned}$$

Similarly as we proved in (2.87), when $N \to \infty$, we have

$$\frac{\Gamma(N-q)}{\Gamma(N)} \sim N^{-q}, \quad \frac{\Gamma(N-q)}{\Gamma(N-1)} \sim N^{-q+1}.$$

Substituting this result into the equation leads to

$$\begin{aligned}
\frac{d^q[x-a]}{[d(x-a)]^q} &= [x-a]^{1-q} \left[\left\{ \lim_{N\to\infty} \frac{N^q}{N^q} \cdot \frac{1}{\Gamma(1-q)} + \lim_{N\to\infty} \frac{N^{q-1}}{N^{q-1}} \cdot \frac{q}{\Gamma(2-q)} \right\} \right] \\
&= [x-a]^{1-q} \left[\left\{ \frac{1}{\Gamma(1-q)} + \frac{q}{\Gamma(2-q)} \right\} \right] \\
&= [x-a]^{1-q} \left[\frac{\Gamma(2-q) + q\Gamma(1-q)}{\Gamma(1-q)\Gamma(2-q)} \right].
\end{aligned}$$

On application of the recurrence property of the Γ function, this leads to

$$\begin{aligned}\frac{d^q[x-a]}{[d(x-a)]^q} &= [x-a]^{1-q}\left[\frac{(1-q)\Gamma(1-q)+q\Gamma(1-q)}{\Gamma(1-q)\Gamma(2-q)}\right] \\ &= [x-a]^{1-q}\left[\frac{\Gamma(1-q)}{\Gamma(1-q)\Gamma(2-q)}\right] \\ &= \frac{[x-a]^{1-q}}{\Gamma(2-q)}.\end{aligned}$$

Alternatively, a similar result can be achieved using the Riemann-Liouville formula (2.41). On substituting $w = x - y$,

$$\begin{aligned}\frac{d^q[x-a]}{[d(x-a)]^q} &= \frac{1}{\Gamma(-q)}\int_a^x \frac{[y-a]}{(x-y)^{q+1}}dy \\ &= \frac{1}{\Gamma(-q)}\int_0^{x-a} \frac{[x-a-w]}{w^{q+1}}dw \\ &= \frac{1}{\Gamma(-q)}\left[\frac{[x-a]^{1-q}}{-q} - \frac{[x-a]^{1-q}}{1-q}\right] \\ &= \frac{[x-a]^{1-q}}{[-q][1-q]\Gamma(-q)}, \quad q < 0.\end{aligned}$$

The denominator of which equals $\Gamma(2-q)$ by applying the recurrence formula

$$-q\Gamma(-q) = \Gamma(1-q) \text{ and } (1-q)\Gamma(1-q) = \Gamma(2-q).$$

Use of equation (2.42) yields

$$\frac{d^{q-n}[x-a]}{[d(x-a)]^{q-n}} = \frac{[x-a]^{1-q+n}}{\Gamma(2-q+n)},$$

where

$$\begin{aligned}\frac{d^q[x-a]}{[d(x-a)]^q} &= \frac{d^n}{[d(x-a)]^q}\left\{\frac{d^{q-n}[x-a]}{[d(x-a)]^{q-n}}\right\} \\ &= \frac{\Gamma(2-q+n)}{\Gamma(2-q)}\frac{[x-a]^{1-q}}{\Gamma(2-q+n)} = \frac{[x-a]^{1-q}}{\Gamma(2-q)},\end{aligned} \tag{2.61}$$

follows by equation (2.36). We note, as expected, that formula (2.61) reduces to zero when $q = 2, 3, 4, \cdots$, to unity when $q = 1$, to $x - a$ when $q = 0$, and to $\dfrac{[x-a]^{n+1}}{(n+1)!}$ when $q = -n = -1, -2, -3 \cdots$. Notice also, on comparison of formulas (2.61) and (2.58), that the q^{th} differintegral of $x - a$ equals the $(q-1)^{th}$ differintegral of unity.

The Function $[x-a]^p$

In this section, we focus on the function $f(x) = [x-a]^p$, where p is initially arbitrary. However, it becomes apparent that p must exceed -1 for differintegration to satisfy the required properties. For integers q of any sign, we can use the classical calculus formula (2.34). Our exploration of non-integer q will initially be limited to negative values, allowing us to leverage the Riemann-Liouville definition.

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{1}{\Gamma(-q)}\int_a^x \frac{[y-a]^p}{[x-y]^{q+1}}dy = \frac{1}{\Gamma(-q)}\int_a^{x-a} \frac{v^p}{[x-a-v]^{q+1}}dv, \quad q<0,$$

where v has replaced $y-a$. By further replacement of v by $[x-a]u$, the integral may be cast into the standard Beta integral form:

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{[x-a]^{p-q}}{\Gamma(-q)}\int_0^1 u^p[1-u]^{-q-1}du, \quad q<0. \tag{2.62}$$

The definite integral in (2.62) is the Beta function (2.2), which is defined as

$$\mathrm{B}\,(p,q) = \int_0^1 y^{p-1}[1-y]^{q-1}dy, \quad p>0<q.$$

Therefore,

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{[x-a]^{p-q}}{\Gamma(-q)}\,\mathrm{B}\,(p+1,-q) = \frac{\Gamma(p+1)[x-a]^{p-q}}{\Gamma(p-q+1)}, \quad q<1, \quad p>-1, \tag{2.63}$$

where the Beta function has been replaced by its Gamma function equivalent using (2.3): $\mathrm{B}\,(p,q) = \dfrac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}$.

Complex variable approach: For comparison of techniques, we verify (2.56) with a completely different approach, starting with the definition (2.48). We replace $x-a$ by z such that

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{d^q z^p}{dz^p} = \frac{\Gamma(q+1)}{2\pi i}\oint_C \frac{\xi^p}{[\xi-z]^{q+1}}d\xi,$$

where the contour C in the complex ξ plane begins and ends at $\xi=0$ enclosing z once in the positive sense. If one sets $\xi = zs$, then

$$\frac{d^q z^p}{dz^p} = \frac{\Gamma(q+1)}{2\pi i} z^{p-q}\oint_C s^p[s-1]^{-q-1}ds,$$

where the integral is over a contour encircling the point $s=1$ once in the positive sense and beginning and ending at $s=0$. When such a contour is deformed into the one shown in Figure

2.1, then

$$\begin{aligned}
\frac{d^q z^p}{dz^p} &= \frac{\Gamma(q+1)z^{p-q}}{2\pi i}\left[1-\exp\left(-2\pi i[q+1]\right)\right]\int_0^1 s^p[s-1]^{-q-1}ds \\
&= \frac{\Gamma(q+1)z^{p-q}}{2\pi i}\exp\left(-i\pi[q+1]\right)\left[\exp\left(i\pi[q+1]\right)-\exp\left(-i\pi[q+1]\right)\right]\int_0^1 s^p[s-1]^{-q-1}ds \\
&= \frac{\Gamma(q+1)z^{p-q}}{2\pi i}[-1]^{[-q-1]}\left[\exp\left(i\pi[q+1]\right)-\exp\left(-i\pi[q+1]\right)\right]\int_0^1 s^p[s-1]^{-q-1}ds \\
&= \frac{\Gamma(q+1)z^{p-q}}{2\pi i}\left[\exp\left(i\pi[q+1]\right)-\exp\left(-i\pi[q+1]\right)\right]\int_0^1 s^p[1-s]^{-q-1}ds \\
&= \frac{\Gamma(q+1)}{2\pi i}z^{p-q}2i\sin\left(\pi[q+1]\right)\int_0^1 s^p[1-s]^{-q-1}ds \\
&= \frac{\Gamma(p+1)z^{p-q}}{\Gamma(p-q+1)}, \quad p>-1, \quad q<0,
\end{aligned}$$

where use has been made of the reflection property of Γ, $\Gamma(z)\Gamma(1-z)=\dfrac{\pi}{\sin(\pi z)}$ and property (2.3) of the Beta integral. We may again use equation (2.42) together with the classical formula (2.36) to extend our treatment to positive q. Following this technique,

$$\begin{aligned}
\frac{d^q[x-a]^p}{[d(x-a)]^q} &= \frac{d^n}{dx^n}\left[\frac{d^{q-n}[x-a]^p}{[d(x-a)]^{q-n}}\right] \\
&= \frac{d^n}{dx^n}\left[\frac{[x-a]^{p-q+n}}{\Gamma(n-q)}\int_0^1 u^p[1-u]^{n-q-1}\,du\right] \\
&= \frac{d^n}{dx^n}\left[\frac{\Gamma(p+1)[x-a]^{p-q+n}}{\Gamma(p-q+n+1)}\right] \\
&= \frac{\Gamma(p+1)}{\Gamma(p-q+n+1)}\frac{d^n}{dx^n}[x-a]^{p-q+n} \\
&= \frac{\Gamma(p+1)}{\Gamma(p-q+n+1)}\frac{\Gamma(p-q+n+1)}{\Gamma(p-q+1)}[x-a]^{p-q} \\
&= \frac{\Gamma(p+1)[x-a]^{p-q}}{\Gamma(p-q+1)}, \quad p>-1.
\end{aligned}$$

where, since we chose $0 \le q < n$, we were able to use (2.58) to evaluate the $[q-n]^{th}$ differintegral of $[x-a]^p$. The classical formula (2.34) then leads to

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{\Gamma(p+1)[x-a]^{p-q}}{\Gamma(p-q+1)}, \quad q\ge 0, \quad p>-1,$$

straightforwardly. Unification of this result with (2.63) yields the formula

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \frac{\Gamma(p+1)[x-a]^{p-q}}{\Gamma(p-q+1)}, \quad p > -1, \tag{2.64}$$

valid for all q. As required for an acceptable formula in our generalized calculus, equation (2.64) incorporates the classical formula (2.35). The formula

$$\frac{d^q x^p}{dx^q} = \frac{\Gamma(p+1)}{\Gamma(p-q+1)} x^{p-q}$$

was important in being the basis of the concept of fractional differentiation as developed by Gemant (1936).

Thus far, this section has only considered instances where $p > -1$ for $[x-a]^p$. We now briefly consider the case where $p \leq -1$. The generalized derivative (2.62) breaks down for $p \leq -1$, because the Beta integrals then diverge. A suggestion of the type

$$\frac{d^q[x-a]^p}{[d(x-a)]^q} = \infty, \quad p \leq -1, \text{all } q,$$

would, however, be unacceptable because it would fail to incorporate the classical result (2.34) for positive integer q. Similarly, formula (2.64) cannot be extended to $p \leq -1$, because although it does not incorporate (2.34), it also does not reproduce (2.35) for negative integer q. Moreover, we know of no generalization of formula (2.64) that incorporates both of the requirements (2.34) and (2.35) for $p \leq -1$. The breakdown of (2.64) for $p \leq -1$ is associated with the pole of order unity or greater which occurs at $x = a$ for the functions $[x-a]^p$, $p \leq -1$. Functions for which such a pole occurs anywhere on the open interval from a to x lead to similar difficulties and for reasons such as this we have purposely excluded these functions from the class of differintegrable series.

2.1.4 General Properties

This chapter delves into the properties of differintegral operators that we anticipate will extend classical formulas for derivatives and integrals. These properties serve as our primary framework for comprehending and employing fractional calculus. While some classical properties generalize seamlessly, others require adjustments. Unless stated otherwise, we presume that all encountered functions are differintegrable as outlined in Section 2.1.2. Throughout this chapter, we often limit our focus to differintegrable series for practical reasons.

Linearity

The linearity of the differintegral operator, by which we mean

$$\frac{d^q[f_1+f_2]}{[d(x-a)]^q} = \frac{d^q f_1}{[d(x-a)]^q} + \frac{d^q f_2}{[d(x-a)]^q}, \tag{2.65}$$

is an immediate consequence of any of the definitions of the differintegral.

Differintegration Term by Term

The linearity of the differintegral operators implies that they can be distributed through the terms of a finite sum; i.e.,

$$\frac{d^q}{[d(x-a)]^q}\sum_{j=0}^{n} f_j = \sum_{j=0}^{n}\frac{d^q f_j}{[d(x-a)]^q}. \tag{2.66}$$

We aim to investigate the circumstances permitting term-by-term differintegration of an infinite series of functions. Our primary objective in this section is to establish the term-by-term differintegrability of general differintegrable series (see Section 2.1.2). We will frequently rely on classical results concerning the differentiation and integration of infinite series term by term (see Section 2.1.1). To utilize these results effectively, we must ensure that the terms f_j of the series are either continuous or continuously differentiable. If we focus on summands f_j that are differintegrable series, the structure of such series and its term-by-term derivative demonstrate that the necessary continuity assumptions hold away from the lower limit $x = a$. Going forward, we will examine infinite sums of differintegrable series and establish results regarding the term-by-term differintegrability of such sums, which will generally hold in open intervals such as $a < x < a + X$, where X represents the radius of convergence of the differintegrable series. First, however, we need to establish some facts about the radius of convergence. Consider first the ordinary power series

$$\phi = \sum_{j=0}^{\infty} c_j [x-a]^j, \quad c_j = \frac{\phi^{(j)}(a)}{j!},$$

convergent for $|x-a| \le X$. One knows from classical results that ϕ, together with all of its term-by-term derivatives and integrals, converges uniformly in the interval $0 \le |x-a| < X$. What can be said about the series obtained, more generally, from term-by-term differintegration of ϕ? Making use of equation (2.64), the series obtained by applying $\dfrac{d^q}{[d(x-a)]^q}$ to every summand of ϕ is the series

$$\sum_{j=0}^{\infty}\frac{c_j\Gamma(j+1)}{\Gamma(j-q+1)}[x-a]^{j-q} = [x-a]^{-q}\sum_{j=0}^{\infty}\frac{\phi^{(j)}(a)}{\Gamma(j-q+1)}[x-a]^j.$$

We know that the series for ϕ converges for $|x-a| < X$, where, by the ratio test,

$$X = \lim_{j\to\infty}\left|\frac{c_j}{c_{j+1}}\right| = \lim_{j\to\infty}\left|\frac{(j+1)\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right|,$$

while the differintegral series will converge for

$$\begin{aligned}
|x-a| &< \lim_{j\to\infty}\left|\frac{\phi^{(j)}(a)\Gamma(j-q+2)}{\phi^{(j+1)}(a)\Gamma(j-q+1)}\right| \\
&= \lim_{j\to\infty}\left|\frac{(j-q+1)\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right| \\
&= \lim_{j\to\infty}\left|\frac{(j+1)\phi^{(j)}(a)}{\phi^{(j+1)}(a)} - \frac{q\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right| \\
&\le \lim_{j\to\infty}\left|\frac{(j+1)\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right| + \Big|-q\Big| \lim_{j\to\infty}\left|\frac{\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right| \\
&= \lim_{j\to\infty}\left|\frac{(j+1)\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right| + |q| \lim_{j\to\infty}\left|\frac{\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right| \\
&= X \pm qA,
\end{aligned}$$

depending on the sign of q, where

$$A = \lim_{j\to\infty}\left|\frac{\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right|.$$

Since q is finite and $j \to \infty$,

$$\begin{aligned}
(j+1) \gg q \quad &\Rightarrow \lim_{j\to\infty}(j+1)\left|\frac{\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right| \gg q \lim_{j\to\infty}\left|\frac{\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right| \\
&\Rightarrow \lim_{j\to\infty}\left|\frac{(j+1)\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right| \gg q \lim_{j\to\infty}\left|\frac{\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right|.
\end{aligned}$$

For $X = \lim_{j\to\infty}\left|\frac{(j+1)\phi^{(j)}(a)}{\phi^{(j+1)}(a)}\right|$, we have $X \gg qA$, which implies that qA is consistently negligible compared to X, indicating that the differintegrated series converges within the open interval $0 < |x-a| < X$. Moreover, the same conclusion applies to the differintegrable series, where the j^{th} term is $c_j[x-a]^{j+p}$ (as this series shares the same radius of convergence as its analytic component, $\sum c_j[x-a]^j$, and thus extends to general differintegrable series). In other words, if the differintegrable series f, which is a finite sum of functions, each representable as

$$[x-a]^p \sum_{j_1=0}^{\infty} c_{j_1}[x-a]^{j_1} + [x-a]^{[np+1]/n} \sum_{j_2=0}^{\infty} c_{j_2}[x-a]^{j_2} + \cdots + [x-a]^{[np+n-1]/n} \sum_{j_n=0}^{\infty} c_{j_n}[x-a]^{j_n},$$

converges for $|x-a| < X$, then so does the series obtained by differintegrating each "unit" term by term, except possibly at the endpoint $x = a$. This fact will be important in what follows. Let f be any differintegrable series. Since f may be decomposed as a finite sum of differintegrable series units,

$$f_v = [x-a]^p \sum_{j=0}^{\infty} c_j [x-a]^j,$$

where $p > -1$ and $c_0 \neq 0$, the term-by-term differintegrability of f will follow from that of f_v. Accordingly, our objective is to establish that

$$\frac{d^q}{[d(x-a)]^q} \left\{ [x-a]^p \sum_{j=0}^{\infty} c_j [x-a]^j \right\} = \sum_{j=0}^{\infty} c_j \frac{d^q [x-a]^{p+j}}{[d(x-a)]^q} \tag{2.67}$$

for all q. More specifically, the equality (2.67) will be proven valid inside the interval of convergence of the differintegrable series $\sum_{j=0}^{\infty} c_j [x-a]^{p+j}$. For $q \leq 0$, a stronger result that directly extends the classical theorem on term-by-term integration is easy to establish as follows. Suppose the infinite series of differintegrable functions $\sum f_j$ converges uniformly in $0 < |x-a| < X$; then

$$\frac{d^q}{[d(x-a)]^q} \sum_{j=0}^{\infty} f_j = \sum_{j=0}^{\infty} \frac{d^q f_j}{[d(x-a)]^q}, \quad q \leq 0, \tag{2.68}$$

and the right-hand series also converges uniformly in $0 < |x-a| < X$. To demonstrate this result, let

$$f = \sum_{j=0}^{\infty} f_j, \quad S_N = \sum_{j=0}^{N} f_j.$$

Since $q < 0$, the Riemann-Liouville representations

$$\frac{d^q f}{[d(x-a)]^q} = \frac{1}{\Gamma(-q)} \int_a^x \frac{f(y)}{[x-y]^{q+1}}\, dy, \quad \frac{d^q f_j}{[d(x-a)]^q} = \frac{1}{\Gamma(-q)} \int_a^x \frac{f_j(y)}{[x-y]^{q+1}}\, dy$$

are valid, and

$$\frac{d^q f}{[d(x-a)]^q} - \frac{d^q S_N}{[d(x-a)]^q} = \frac{1}{\Gamma(-q)} \int_a^x \frac{[f(y) - S_N]}{[x-y]^{q+1}}\, dy.$$

The property of uniform convergence means that, given $\epsilon > 0$, there is an integer $N = N(\epsilon)$ such that

$$|f(y) - S_n(y)| < \epsilon,$$

for $n > N$ and for all y in the interval $a \le y \le x$ with $|x-a| < X$. Then

$$\begin{aligned}
\left|\frac{d^q f}{[d(x-a)]^q} - \frac{d^q f_j}{[d(x-a)]^q}\right| &= \frac{1}{\Gamma(-q)}\left|\int_a^x \frac{[f(y)-S_N]}{[x-y]^{q+1}}\,dy\right| \\
&\le \frac{1}{\Gamma(-q)}\int_a^x \frac{|f(y)-S_N(y)|dy}{[x-y]^{q+1}} \\
&< \frac{\epsilon}{\Gamma(-q)}\int_a^x [x-y]^{-q-1}dy \\
&= \frac{\epsilon[x-a]^{-q}}{q\Gamma(-q)} \\
&< \frac{\epsilon X^{-q}}{q\Gamma(-q)},
\end{aligned}$$

which can be made small, with $\epsilon \to 0$, independently of x, in the interval $0 < |x-a| < X$. This proves that $\sum \frac{d^q f_j}{[d(x-a)]^q}$ converges uniformly to $\frac{d^q f}{[d(x-a)]^q}$ in $0 < |x-a| < X$. The result just established shows that equation (2.67) is valid for $q \le 0$, and thus, if f is any differintegrable series, the operator $\frac{d^q}{[d(x-a)]^q}$ may be distributed through the several infinite series that define f as long as $q \le 0$.

Applying result (2.64) to equation (2.67) gives

$$\frac{d^q f_v}{[d(x-a)]^q} = \sum_{j=0}^{\infty} \frac{c_j\Gamma(p+j+1)}{\Gamma(p-q+j+1)}[x-a]^{p+j-q}, \quad q \le 0. \tag{2.69}$$

Equations (2.67) and (2.69) are also valid for $q > 0$, as we now establish. First, we decompose the series for f_v into two expressions:

$$f_v = \sum_{j=0}^{\infty} c_j[x-a]^{p+j} = \sum_{j\in J_1} c_j[x-a]^{p+j} + \sum_{j\in J_2} c_j[x-a]^{p+j},$$

where J_1 is the set of nonnegative integers j for which $\Gamma(p-q+j+1)$ is infinite, and J_2 consists of all nonnegative integers not in J_1. $\Gamma(p-q+j+1)$ being infinite implies that $p-q+j+1$ is either zero or a negative integer. However, as j increases, and since $p-q+1$ is finite, $p-q+1+j$ is guaranteed to become greater than zero for finite values of j. This implies that the values of j for which $p-q+1+j$ can be either negative or zero are also finite. Therefore, J_1 is finite.

$$\begin{aligned}
\frac{d^q f_v}{[d(x-a)]^q} &= \frac{d^q}{[d(x-a)]^q}\left\{\sum_{j\in J_1} c_j[x-a]^{p+j}\right\} + \frac{d^q}{[d(x-a)]^q}\left\{\sum_{j\in J_2} c_j[x-a]^{p+j}\right\} \\
&= \sum_{j\in J_1} \frac{d^q[x-a]^{p+j}}{[d(x-a)]^q} + \frac{d^q}{[d(x-a)]^q}\left\{\sum_{j\in J_2} c_j[x-a]^{p+j}\right\},
\end{aligned}$$

making use only of the linearity of $\dfrac{d^q}{[d(x-a)]^q}$. Now we see that the proof of equation (2.69) for $q > 0$ depends only upon establishing that

$$\frac{d^q}{[d(x-a)]^q}\left\{\sum_{j\in J_2} c_j[x-a]^{p+j}\right\} = \sum_{j\in J_2} c_j\frac{d^q[x-a]^{p+j}}{[d(x-a)]^q} = \sum_{j\in J_2}\frac{c_j\Gamma(p+j+1)}{\Gamma(p-q+j+1)}[x-a]^{p+j-q}, \quad q>0. \tag{2.70}$$

Given the uniform convergence of the series for f_v in $0 < |x-a| < X$, the series on the right-hand side of equation (2.70) will also converge uniformly, as demonstrated earlier in this section. Hence, the operator $\dfrac{d^{-1}}{[d(x-a)]^{-1}}$ can be applied to the terms of this series to obtain

$$\begin{aligned}
&\frac{d^{-1}}{[d(x-a)]^{-1}}\left\{\sum_{j\in J_2}\frac{c_j\Gamma(p+j+1)}{\Gamma(p-q+j+1)}[x-a]^{p+j-q}\right\}\\
&=\sum_{j\in J_2}\frac{d^{-1}}{[d(x-a)]^{-1}}\left\{\frac{c_j\Gamma(p+j+1)}{\Gamma(p-q+j+1)}[x-a]^{p+j-q}\right\}\\
&=\sum_{j\in J_2}\frac{c_j\Gamma(p+j+1)\Gamma(p-q+j+1)}{\Gamma(p-q+j+1)\Gamma(p-q+j+2)}[x-a]^{p+j-q+1}\\
&=\sum_{j\in J_2}\frac{c_j\Gamma(p+j+1)}{\Gamma(p-q+j+2)}[x-a]^{p+j-q+1}\\
&=\sum_{j\in J_2}c_j\frac{d^{q-1}}{[d(x-a)]^{q-1}}[x-a]^{p+j}.
\end{aligned} \tag{2.71}$$

Moreover, the last series converges uniformly in $0 < |x-a| < X$, as does the series obtained by differentiating each term. The cancellation required to derive the penultimate expression in equation (2.71) can be justified since the definition of set J_2 ensures that $\Gamma(p-q+j+1)$ is finite. Applying the classical theorem on term-by-term differentiation (see Section 2.1.1) to the series $\sum c_j\dfrac{d^{q-1}}{[d(x-a)]^{q-1}}[x-a]^{p+j}$ yields

$$\frac{d}{dx}\left\{\sum_{j\in J_2}c_j\frac{d^{q-1}}{[d(x-a)]^{q-1}}[x-a]^{p+j}\right\} = \sum_{j\in J_2}c_j\frac{d^q}{[d(x-a)]^q}[x-a]^{p+j}.$$

Arguing similarly, we find that

$$\frac{d^n}{dx^n}\left\{\sum_{j\in J_2}c_j\frac{d^{q-n}}{[d(x-a)]^{q-n}}[x-a]^{p+j}\right\} = \sum_{j\in J_2}c_j\frac{d^q}{[d(x-a)]^q}[x-a]^{p+j}, \tag{2.72}$$

for every positive integer n. Choosing the smallest n to make $q - n < 0$ permits us to apply equation (2.69) with the result that

$$\sum_{j \in J_2} c_j \frac{d^{q-n}}{[d(x-a)]^{q-n}} [x-a]^{p+j} = \frac{d^{q-n}}{[d(x-a)]^{q-n}} \left\{ \sum_{j \in J_2} c_j [x-a]^{p+j} \right\}.$$

Differentiating both sides of this equation n times, we see that

$$\frac{d^n}{dx^n} \left\{ \sum_{j \in J_2} c_j \frac{d^{q-n}}{[d(x-a)]^{q-n}} [x-a]^{p+j} \right\} = \frac{d^q}{[d(x-a)]^q} \left\{ \sum_{j \in J_2} c_j [x-a]^{p+j} \right\}.$$

Utilizing equation (2.72) gives, finally,

$$\frac{d^q}{[d(x-a)]^q} \left\{ \sum_{j \in J_2} c_j [x-a]^{p+j} \right\} = \sum_{j \in J_2} c_j \frac{d^q}{[d(x-a)]^q} [x-a]^{p+j}, \quad q > 0,$$

as we wanted to show. Thus the representation (2.70) is valid for $q > 0$ and, hence, for arbitrary q.

Scale Change

By a scale change of the function f with respect to a lower limit a, we mean its replacement by $f(\beta - \beta + a)$, where β is a constant termed the scaling factor. To clarify this definition, consider $a = 0$; then the scale change converts $f(x)$ to $f(\beta x)$, in contrast to the homogeneity operation to the previous section which converted $f(x)$ to $Cf(x)$.

In this section we seek a procedure by which the effect to the generalized $\dfrac{d^q}{[d(x-a)]^q}$ operation upon $f(\beta x - \beta a + a)$ can be found, if $\dfrac{d^q}{[d(x-a)]^q}$ is known. We shall find it convenient to use the abbreviation

$$X = x + [a - a\beta]/\beta,$$

and to adopt the Riemann-Liouville definition (2.41). Using Y as a replacement for $\beta y - \beta a + a$, we proceed as follows:

$$\begin{aligned}
\frac{d^q f(\beta X)}{[d(x-a)]^q} = \frac{d^q f(\beta y - \beta a + a)}{[d(x-a)]^q} &= \frac{1}{\Gamma(-q)} \int_a^x \frac{f(\beta y - \beta a + a)}{[x-y]^{q+1}} dy \\
&= \frac{1}{\Gamma(-q)} \int_a^{\beta x} \frac{f(Y)[dY/\beta]}{[\beta X - Y]/\beta^{q+1}} \\
&= \frac{\beta^q}{\Gamma(-q)} \int_a^{\beta X} \frac{f(Y)}{[\beta X - Y]^{q+1}} dY \\
&= \beta^q \frac{d^q f(\beta X)}{[d(\beta X - a)]^q}.
\end{aligned} \tag{2.73}$$

The unity of the formula (2.73) is greatest when $a = 0$, for then $X = x$ and the scale change is simply a multiplication of the independent variable by a constant, the formula being

$$\frac{d^q f(\beta X)}{[dx]^q} = \beta^q \frac{d^q f(\beta X)}{[d\beta x]^q}. \tag{2.74}$$

Leibniz's Rule

The rule for differentiating a product of two functions is a well-known result in elementary calculus. It states that

$$\frac{d^n[fg]}{dx^n} = \sum_{j=0}^{n} \binom{n}{j} \frac{d^{n-j} f}{dx^{n-j}} \frac{d^j g}{dx^j} \tag{2.75}$$

and is, of course, limited to non-negative integers n. In Section 2.1.1, we derived, employing integration by parts, the subsequent product rule for multiple integrals:

$$\frac{d^{-n}[fg]}{[d(x-a)]^{-n}} = \sum_{j=0}^{\infty} \binom{-n}{j} \frac{d^{-n-j} f}{[d(x-a)]^{-n-j}} \frac{d^j g}{[d(x-a)]^j}.$$

When we observe that the finite sum in (2.75) could equally well extend to infinity [since $\binom{n}{j} = 0$ for $j > n$], we might expect the product rule to generalize to arbitrary order q as

$$\frac{d^q[fg]}{[d(x-a)]^q} = \sum_{j=0}^{\infty} \binom{q}{j} \frac{d^{q-j} f}{[d(x-a)]^{-q-j}} \frac{d^j g}{[d(x-a)]^j}. \tag{2.76}$$

That such generalization is indeed valid for real analytic functions $\phi(x)$ and $\psi(x)$ will now be established.
Starting with equation (2.60) and substituting for ϕ the product $\phi\psi$, we obtain

$$\begin{aligned} \frac{d^q[\phi\psi]}{[d(x-a)]^q} &= \sum_{k=0}^{\infty} \binom{q}{k} \frac{d^{q-k}[1]}{[d(x-a)]^{q-k}} [\phi\psi]^{(k)} \\ &= \sum_{k=0}^{\infty} \binom{q}{k} \frac{d^{q-k}[1]}{[d(x-a)]^{q-k}} \sum_{j=0}^{k} \binom{k}{j} \phi^{(k-j)} \psi^{(j)}, \end{aligned}$$

making use of (2.75). Note that, since j is an integer, the repeated derivative $\psi^{(j)}$ with respect to x equals that with respect to $x - a$. The permutation (2.94)

$$\sum_{k=0}^{\infty} \sum_{j=0}^{k} = \sum_{j=0}^{\infty} \sum_{k=j}^{\infty} \tag{2.77}$$

may be applied to give

$$\begin{aligned}\frac{d^q[\phi\psi]}{[d(x-a)]^q} &= \sum_{j=0}^{\infty}\psi^{(j)}\sum_{k=j}^{\infty}\binom{q}{k}\binom{k}{j}\frac{d^{q-k}[1]}{[d(x-a)]^{q-k}}\phi^{(k-j)}\\ &= \sum_{j=0}^{\infty}\psi^{(j)}\sum_{l=0}^{\infty}\binom{q}{l+j}\binom{l+j}{j}\frac{d^{q-j-l}[1]}{[d(x-a)]^{-q-j-l}}\phi^{(l)}\\ &= \sum_{j=0}^{\infty}\binom{q}{j}\psi^{(j)}\sum_{l=0}^{\infty}\binom{q-j}{l}\frac{d^{q-j-l}[1]}{[d(x-a)]^{-q-j-l}}\phi^{(l)}\\ &= \sum_{j=0}^{\infty}\psi^{(j)}\binom{q}{j}\frac{d^{q-j}[1]}{[d(x-a)]^{-q-j}}\phi,\end{aligned}$$

where we have made use of the identity (2.95)

$$\binom{q}{l+j}\binom{l+j}{j} = \binom{q}{j}\binom{q-j}{l},$$

the proof of which can be found in subsection 2.1.5, and the subsequent application of (2.60). We established (2.55) under the assumption that ϕ is a real analytic function and utilized (2.55) to demonstrate (2.60), which, in turn, was employed to establish (2.76). Therefore, the latter is proven only if both ϕ and ψ are real analytic functions.

Composition Rule

In our quest for a comprehensive composition rule for the operator $\dfrac{d^q}{[d(x-a)]^q}$, we aim to uncover the connection between

$$\frac{d^q}{[d(x-a)]^q}\cdot\frac{d^Q}{[d(x-a)]^Q}, \quad \text{and} \quad \frac{d^{q+Q}}{[d(x-a)]^{q+Q}},$$

which we temporarily abbreviate to $d^q d^Q f$ and d^{q+Q} respectively. Naturally, for these symbols to have general significance, we must assume not only that f is differintegrable but also that $d^Q f$ is differintegrable. In this section, we confine our focus to differintegrable series as defined in Section 2.1.2. Thereby, the most general non-zero differintegrable series is a finite sum of differintegrable "units," each taking the form

$$f_v = [x-a]^p\sum_{j=0}^{\infty}c_j[x-a]^j, \quad p > -1, \quad c_0 \neq 0. \tag{2.78}$$

We shall see that the composition rule may be valid for some units of f but possibly not for others. It follows from the linearity of differintegral operators that

$$d^q d^Q f = d^{q+Q} f \tag{2.79}$$

if

$$d^q d^Q f_v = d^{q+Q} f_v \tag{2.80}$$

for every unit f_v of f. Accordingly, we shall first assess the validity of the composition rule (2.80) for differintegrable series unit functions f_v. Obviously, if $f_v \equiv 0$, then $d^Q f_v = 0$ for every Q by equation (2.57), and so

$$d^q d^Q [0] = d^{q+Q}[0] = 0.$$

While the composition rule is trivially satisfied for the differintegrable function $f_v \equiv 0$, we shall see that the possibility

$$f_v \neq 0, \quad \text{but} \quad d^Q f_v = 0,$$

is exactly the condition that prevents the composition rule (2.80), and therefore (2.79), from being satisfied generally. Having dealt with the case $f_v \equiv 0$, we now assume $f_v \neq 0$ and use equation (2.69) to evaluate $d^Q f_v$:

$$d^Q f_v = \sum_{j=0}^{\infty} c_j d^Q [x-a]^{p+j} = \sum_{j=0}^{\infty} \frac{c_j \Gamma(p+j+1)[x-a]^{p+j-Q}}{\Gamma(p+j-Q+1)}. \tag{2.81}$$

Furthermore, we observe that since $p > -1$, it implies that $p + j > -1$, ensuring that $\Gamma(p+j+1)$ is always finite but nonzero. Hence, individual terms in $d^Q f_v$ will only vanish when the coefficient c_j is zero or when the denominatorial Γ function $\Gamma(p+j+1-Q)$ is infinite. Consequently, we realize that a necessary and sufficient condition for $d^Q f_v \neq 0$ is

$$\Gamma(p+j+1-Q) \quad \text{is finite for each} \quad j \quad \text{for which} \quad c_j \neq 0. \tag{2.82}$$

This awkward condition (2.82) may be shown to be equivalent to

$$f_v - d^{-Q} d^Q f_v = 0; \tag{2.83}$$

that is, to the condition that the differintegrable unit f_v be regenerated upon the application, first of d^Q, then d^{-Q}. Assuming (2.83) temporarily, we find that d^q may then be applied to equation (2.81) to give

$$d^q d^Q f_v = \sum_{j=0}^{\infty} \frac{c_j \Gamma(p+j+1)\Gamma(p+j-Q+1)[x-a]^{p+j-Q-q}}{\Gamma(p+j-Q+1)\Gamma(p+j-Q-q+1)}.$$

On the other hand, the same technique shows that

$$d^{q+Q} f_v = \sum_{j=0}^{\infty} c_j d^{q+Q} f_v = \sum_{j=0}^{\infty} \frac{c_j \Gamma(p+j+1)[x-a]^{p+j-Q-q}}{\Gamma(p+j-Q-q+1)} = d^q d^Q f_v.$$

Thus, the composition rule (2.80) is obeyed for the unit f_v as long as condition (2.83) is satisfied. However, when (2.83) is violated, $d^Q f_v = 0$ so that $d^q d^Q f_v = 0$. On the other hand, it is not necessarily the case that $d^{q+Q}f_v = 0$. For example, we may choose $f_v = x^{-1/2}$, $a = 0$, $Q = \frac{1}{2}$, and $q = -\frac{1}{2}$. Then

$$f_v - d^{-Q}d^{Q}f_v = x^{-1/2} - d^{-1/2}d^{1/2}x^{-1/2} = x^{-1/2} - d^{-1/2}\frac{\Gamma(\frac{1}{2})}{\Gamma(0)}x^{-1/2} = x^{-1/2} \neq 0,$$

so that condition (2.83) is certainly violated. Therefore, $d^{Q}f_v = 0$ and $d^{q}d^{Q}f_v = 0$ while $d^{q+Q}f_v = x^{-1/2} \neq 0$. Generalizing, we easily see the relationship between $d^{q}d^{Q}f_v$ and $d^{q+Q}f_v$ in case $f_v - d^{-Q}d^{Q}f_v \neq 0$ to be

$$0 = d^{q}d^{Q}f_v = d^{q+Q}f_v - d^{q+Q}\{f_v - d^{-Q}d^{Q}f_v\}. \tag{2.84}$$

The preceding discussion for differintegrable units f_v is summarized in the Table 2.1.

	$f_v \equiv 0$	$f_v \neq 0$
$d^{Q}f_v = 0$	$f_v - d^{-Q}d^{Q}f_v = 0$ $d^{q}d^{Q}f_v = d^{q+Q}f_v = 0$	$f_v - d^{-Q}d^{Q}f_v \neq 0$ $0 = d^{q}d^{Q}f_v = d^{q+Q}f_v$ $- d^{q+Q}[f_v - d^{-Q}d^{Q}f_v]$
$d^{Q}f_v \neq 0$	Not attainable	$f_v - d^{-Q}d^{Q}f_v = 0$ $d^{q}d^{Q}f_v = d^{q+Q}f_v.$

Table 2.1: Summary of the composition rule for differintegrable units f_v

While equation (2.84) is a trivial identity for differintegrable units, its significance becomes more apparent and thus more useful for general differintegrable series. Because equation (2.79) holds true for general differintegrable series f if and only if equation (2.80) is valid for every differintegrable unit f_v of f, applying the theory developed for units f_v to derive the composition rule for general f is straightforward. The only difference lies in the conditions

$$f_v \neq 0 \quad \text{and} \quad f_v - d^{-Q}d^{Q}f_v = 0 \tag{2.85}$$

for units f_v guaranteed that $d^{Q}f_v \neq 0$, this is no longer the case for arbitrary f. The reason, of course, is that some units of f may satisfy (2.85) while others do not. This will make it possible to violate the composition rule (2.79) even though

$$f \neq 0 \quad \text{and} \quad d^{Q}f \neq 0.$$

Then, in conjunction with the preceding requirement, it is imperative to include an additional condition

$$f_v - d^{-Q}d^{Q}f_v = 0 \tag{2.86}$$

for each differintegrable unit, as delineated in Table 2.2.

Note:

Section 2.1.5 provides proofs for certain results utilized in Chapter 2. If these have been previously reviewed, the reader should then proceed to Chapter 3.

	$f \equiv 0$	$f \neq 0$
$d^{Q}f \equiv 0$	$f - d^{-Q}d^{Q}f \equiv 0$ $d^{q}d^{Q}f = d^{q+Q}f = 0$	$f - d^{-Q}d^{Q}f \neq 0$ $0 = d^{q}d^{Q}f = d^{q+Q}f$ $- d^{q+Q}[f - d^{-Q}d^{Q}f]$
$d^{Q}f \neq 0$	Not attainable	if $f - d^{-Q}d^{Q}f \equiv 0$ then $d^{q}d^{Q}f = d^{q+Q}f$ if $f - d^{-Q}d^{Q}f \neq 0$ then $d^{q}d^{Q}f = d^{q+Q}f$ $- d^{q+Q}[f - d^{-Q}d^{Q}f]$.

Table 2.2: Summary of the composition rule for arbitrary differintegrable functions, f.

2.1.5 Auxiliary Proofs

The following properties, along with their accompanying proofs, were frequently utilized to derive important results in this chapter:

1. We aim to prove

$$\lim_{j\to\infty}\left[j^{c+q+1}\frac{\Gamma(j-q)}{\Gamma(j+1)}\right] = \lim_{j\to\infty}\left[j^{c+q}\frac{\Gamma(j-q)}{\Gamma(j)}\right] = \begin{cases}\infty, & c>0,\\ 1, & c=0,\\ 0, & c<0\end{cases} \tag{2.87}$$

Given that $\lim_{j\to\infty}\left[j^{c+q+1}\frac{\Gamma(j-q)}{\Gamma(j+1)}\right] = \lim_{j\to\infty}\left[j^{c+q}\frac{\Gamma(j-q)}{\Gamma(j)}\right]$. Using the asymptotic expansion of $\dfrac{\Gamma(j-q)}{\Gamma(j+1)}$ (2.1), we have

$$\frac{\Gamma(j-q)}{\Gamma(j+1)} \sim j^{-1-q}\left[1+\frac{q[q+1]}{2j}+\mathcal{O}(j^{-2})\right], \quad q \in \mathbb{R}, \quad j \in \mathbb{N}, \quad \text{and} \quad j \to \infty.$$

Subsequently,

$$\frac{\Gamma(j-q)}{\Gamma(j+1)} = \frac{\Gamma(j-q)}{j\Gamma(j)} \Rightarrow \frac{\Gamma(j-q)}{\Gamma(j)} \sim j^{-q}\left[1+\frac{q[q+1]}{2j}+\mathcal{O}(j^{-2})\right].$$

Additionally,

$$j \to \infty \Rightarrow \frac{q[q+1]}{2j} \to 0 \Rightarrow \frac{\Gamma(j-q)}{\Gamma(j)} \sim j^{-q}.$$

Applying this result in (2.87) leads to

$$\lim_{j\to\infty}\left[j^{c+q}\frac{\Gamma(j-q)}{\Gamma(j)}\right] = \lim_{j\to\infty}\frac{j^{c+q}}{j^q} = \lim_{j\to\infty} j^c = \begin{cases} \infty, & c>0, \\ 1, & c=0, \\ 0, & c<0. \end{cases} \tag{2.88}$$

2. We aim to prove that

$$[-1]^j\binom{n}{j} = \binom{j-n-1}{j} = \frac{\Gamma(j-n)}{\Gamma(-n)\Gamma(j+1)}. \tag{2.89}$$

Let Q_1 be $[-1]^j\binom{n}{j}$, Q_2 $\binom{j-n-1}{j}$ and Q_3 be $\dfrac{\Gamma(j-n)}{\Gamma(-n)\Gamma(j+1)}$. In order to derive that proof, we show that both Q_1 and Q_2 are equal to Q_3 .
Let us first show that Q_2 are equal to Q_3.

$$Q_2 = \binom{j-n-1}{j} = \frac{\Gamma(j-n)}{\Gamma(j+1)\Gamma(-n)}.$$

Let us now show that Q_1 are equal to Q_3

$$Q_1 = [-1]^j\binom{n}{j} = [-1]^j\frac{\Gamma(n+1)}{\Gamma(n-j+1)\Gamma(j+1)}.$$

From the previous result, we only need to show that

$$[-1]^j\frac{\Gamma(n+1)}{\Gamma(n-j+1)} = \frac{\Gamma(j-n)}{\Gamma(-n)}.$$

On one hand, using the reflection property of Γ, and the fact that $\cos(j\pi) = [-1]^j$ for all positive integers j, we have

$$\begin{aligned}
\Gamma(j-n) = \Gamma\left(-(n-j)\right) &= \frac{-\pi}{\sin((n-j)\pi)\Gamma(n-j+1)} \\
&= \frac{-\pi}{\Gamma(n-j+1)\left(\sin(\pi n)\cos(\pi j) - \cos(\pi n)\sin(\pi j)\right)} \\
&= \frac{-\pi}{\Gamma(n-j+1)\sin(\pi n)[-1]^j}.
\end{aligned}$$

On the other hand, taking advantage of the reflection property again, we have

$$\Gamma(-n) = \frac{-\pi}{\Gamma(n+1)\sin(\pi n)}.$$

Finally, using the former results, we have

$$\begin{aligned}
\frac{\Gamma(j-n)}{\Gamma(-n)} &= \frac{-\pi}{\Gamma(n-j+1)\sin(\pi n)[-1]^j}\ \frac{\Gamma(n+1)\sin(\pi n)}{-\pi} \\
&= \frac{\Gamma(n+1)[-1]^{-j}}{\Gamma(j-j+1)} \\
&= [-1]^j \frac{\Gamma(n+1)}{\Gamma(n-j+1)}.
\end{aligned}$$

3. Let us establish that

$$\sum_{j=0}^{n} \binom{j-q-1}{j} = \binom{n-q}{n}. \tag{2.90}$$

We aim to show using induction that $\forall n \in \mathbb{N}$,

$$\sum_{j=0}^{n} \binom{j-q-1}{j} = \binom{n-q}{n}.$$

Initial condition: $n = 1$. The left hand side of the equation gives

$$\sum_{j=0}^{1} \binom{j-q-1}{j} = \binom{0-1-q}{0} + \binom{1-q-1}{1} = \binom{-q-1}{0} + \binom{-q}{1} = 1-q.$$

The right hand side of the equation gives

$$\binom{1-q}{1} = 1-q.$$

Let us suppose now the equation is true for $n = k$ and let us prove that it is also true for $n = k+1$. We need to show that

$$\sum_{j=0}^{k+1} \binom{j-q-1}{j} = \binom{k+1-q}{k+1}.$$

$$\begin{aligned}
\sum_{j=0}^{k+1} \binom{j-q-1}{j} &= \sum_{j=0}^{k} \binom{j-q-1}{j} + \binom{k+1-q-1}{k+1} \\
&= \sum_{j=0}^{k} \binom{j-q-1}{j} + \binom{k-q}{k+1} \\
&= \binom{k-q}{k} + \binom{k-q}{k+1}.
\end{aligned}$$

$$\binom{k-q}{k} = \frac{\Gamma(k-q+1)}{\Gamma(k+1)\Gamma(-q+1)} = \frac{\Gamma(k-q+1)}{\Gamma(k+1)(-q)\Gamma(-q)}.$$

$$\binom{k-q}{k+1} = \frac{\Gamma(k-q+1)}{\Gamma(k+2)\Gamma(-q)} = \frac{\Gamma(k-q+1)}{(k+1)\Gamma(k+1)\Gamma(-q)}.$$

$$\begin{aligned}
\binom{k-q}{k} + \binom{k-q}{k+1} &= \frac{\Gamma(k-q+1)}{\Gamma(k+1)(-q)\Gamma(-q)} + \frac{\Gamma(k-q+1)}{(k+1)\Gamma(k+1)\Gamma(-q)} \\
&= \frac{1}{\Gamma(k+1)\Gamma(-q)} \left\{ \frac{\Gamma(k-q+1)}{-q} + \frac{\Gamma(k-q+1)}{k+1} \right\} \\
&= \frac{\Gamma(k-q+1)(k+1-q)}{(-q)\Gamma(k+1)\Gamma(-q)(k+1)} = \frac{\Gamma(k-q+2)}{\Gamma(-q+1)\Gamma(k+2)} \\
&= \binom{k-q+1}{k+1}.
\end{aligned}$$

4. Let us prove that

$$\sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)} = \frac{\Gamma(N-q)}{\Gamma(1-q)\Gamma(N)}. \tag{2.91}$$

This result is derived by setting $N = n+1$ and expressing the binomial coefficients as their equivalent Γ function combination in (2.90) as follows:

$$\sum_{j=0}^{n} \binom{j-q-1}{j} = \binom{n-q}{n} \Leftrightarrow \sum_{j=0}^{n} \frac{\Gamma(j-q)}{\Gamma(j+1)\Gamma(-q)} = \frac{\Gamma(n-q+1)}{\Gamma(n+1)\Gamma(-q+1)}.$$

By setting $N = n+1$, we obtain

$$\sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)\Gamma(-q)} = \frac{\Gamma(N-q)}{\Gamma(N)\Gamma(1-q)}.$$

5. Our purpose is to demonstrate that

$$\sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j)} = \frac{-q\Gamma(N-q)}{\Gamma(2-q)\Gamma(N-1)}. \tag{2.92}$$

For this proof, let us consider the following binomial coefficient identity which can also be verified using induction as shown in (2.90).

$$\sum_{j=1}^{n} \binom{j-q-1}{j-1} = \binom{n-q}{n-1} \Leftrightarrow \sum_{j=1}^{n} \frac{\Gamma(j-q)}{\Gamma(j)\Gamma(-q+1)} = \frac{\Gamma(n-q+1)}{\Gamma(n)\Gamma(2-q)}.$$

By setting $N = n+1$, we obtain, this finally leads to

$$\sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j)\Gamma(-q+1)} = \frac{\Gamma(N-q)}{\Gamma(N-1)\Gamma(2-q)}.$$

Using the recurrence property of the Γ function leads to

$$\sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j)(-q)\Gamma(-q)} = \frac{\Gamma(N-q)}{\Gamma(N-1)\Gamma(2-q)} \Leftrightarrow \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j)\Gamma(-q)} = \frac{-q\Gamma(N-q)}{\Gamma(N-1)\Gamma(2-q)}.$$

6. Let us establish the binomial result

$$\sum_{k=0}^{j} \binom{q}{k}\binom{Q}{j-k} = \binom{q+Q}{j}. \tag{2.93}$$

For q and Q intergers, this equality implies that choosing j elements out of $q+Q$ elements, i.e., $\binom{q+Q}{j}$, is equivalent to choosing k elements out of q, i.e., $\binom{q}{k}$, and $j-k$ elements out of Q, i.e., $\binom{Q}{j-k}$. Finally, by considering all the possible values of k between 0 and j, we obtain the desired result.

For q and Q reals numbers, we have

$$\sum_{j=0}^{\infty} \binom{q+Q}{j} x^j = (1+x)^{q+Q} = (1+x)^q(1+x)^Q = \Big(\sum_{k=0}^{\infty} \binom{q}{k} x^q\Big)\Big(\sum_{l=0}^{\infty} \binom{Q}{l} x^Q\Big).$$

Upon applying the summation formula

$$\sum_{n=0}^{\infty} a_n \sum_{n=0}^{\infty} b_n = \sum_{n=0}^{\infty}\sum_{k=0}^{n} a_k b_{n-k},$$

we obtain

$$\sum_{j=0}^{\infty} \binom{q+Q}{j} x^j = (1+x)^{q+Q} = \sum_{j=0}^{\infty} \left(\sum_{k=0}^{j} \binom{q}{k} \binom{Q}{j-k} \right) x^j$$
$$\Leftrightarrow \binom{q+Q}{j} = \sum_{k=0}^{j} \binom{q}{k} \binom{Q}{j-k}.$$

7. We aim to establish the binomial equality

$$\binom{q}{l+j} \binom{l+j}{j} = \binom{q}{j} \binom{q-j}{l}. \tag{2.94}$$

A good way to understand this binomial equality is to consider the example of a box containing q balls. Out of those q balls, such that we have l which are red and j which are blue. This equality represents 2 identical ways to choose those l red balls and j blue balls out of those q balls. The first way (the left-hand side) involves selecting $l + j$ balls then, assigning l to be red and j to be blue (a total of $l + j$) all at once out of the q balls $\binom{q}{l+j}$. Subsequently, out of the $(l + j)$ selected, we select either j blue balls or l red balls since $\binom{l+j}{j} = \binom{l+j}{l}$. The second way (the right-hand side) consists of selecting each color ball one after the other. We first choose the j red ones out of the q total $\binom{q}{j}$. Then, out of the $q - j$ balls remaining, we select the blue ones $\binom{q-j}{l}$.

8.
$$\sum_{k=0}^{\infty} \sum_{j=0}^{k} = \sum_{j=0}^{\infty} \sum_{k=j}^{\infty}. \tag{2.95}$$

The summation equality is established graphically:
$\sum_{k=0}^{\infty} \sum_{j=0}^{k}$ is the discrete equivalent to the double integral $\int_0^{\infty} \int_0^{x} dy\ dx$, which represents the area of the lower region delimited by the x-axis, the y-axis, and the line $y = x$, as shown in Figure 2.2 (red). Similarly, $\sum_{j=0}^{\infty} \sum_{k=j}^{\infty}$ is the discrete equivalent to the double integral $\int_0^{\infty} \int_y^{\infty} dx\ dy$, representing the area of the upper region delimited by the x-axis, the y-axis, and the line $y = x$, as shown in Figure 2.2 (black). From Figure 2.2, these areas are equal, and then, (g) follows.

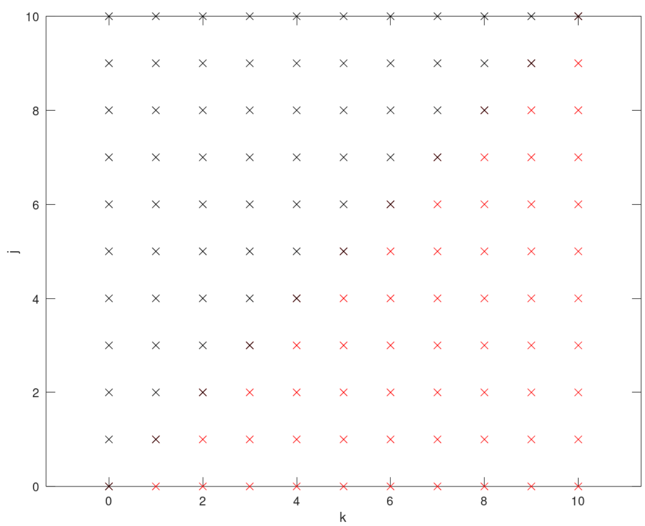


Figure 2.2: Upper and lower regions of equal areas.

The discret version of this proof involves $\sum_{k=0}^{\infty}\sum_{j=0}^{k}$ sums over all pairs (k, j) where $j \leq k$, and $\sum_{j=0}^{\infty}\sum_{k=j}^{\infty}$ sums over all pairs (k, j) where $k \geq j$.

Chapter 3

Gierer-Meinhardt Model

3.1 Representation, Matched Asymptotic Expansion and Solution

Our study will focus solely on sub-diffusion with Gierer-Meinhardt reaction kinetics. The Gierer-Meinhardt model is a mathematical model that describes the formation of spatial patterns in biological systems. Proposed by Hans Meinhardt and Leo Gierer in the late 1960s, the model studies the interaction between the activator and the inhibitor. The original Gierer-Meinhardt model is represented by a system of two partial differential equations characterizing the rate of change of the concentrations of both activator and inhibitor species with respect to space and time:

$$\partial_t a = \epsilon^2 a_{xx} - a + \frac{a^p}{h^q}, \quad \tau \partial_t h = D h_{xx} - h + \epsilon^{-1} \frac{a^m}{h^s}, \tag{3.1}$$

where $a(x,t)$ and $h(x,t)$ are the activator and inhibitor concentrations at position x and time t. Here ϵ^2 and D denote the constant diffusivities, τ is the reaction time constant, and the exponents (p, q, m, s) satisfy

$$p > 1,\ q > 0,\ m > 0,\ s \geq 0,\ \frac{p-1}{q} < \frac{m}{s+1}.$$

When integrating sub-diffusion into the system, involving some concepts of fractional calculus, we obtain the following system

$$\partial_t^\gamma a = \epsilon^{2\gamma} a_{xx} - a + \frac{a^p}{h^q}, \quad \tau \partial_t^\gamma h = D h_{xx} - h + \epsilon^{-\gamma} \frac{a^m}{h^s}, \tag{3.2}$$

where the anomaly exponent γ is in the range $0 < \gamma < 1$. The original Gierer-Meinhardt model can be recovered by substituting $\gamma = 1$ in the new system (3.2). Setting $\gamma \to 0^+$

is inappropriate since ϵ^{γ} becomes arbitrarily small as $\epsilon \to 0$ when $0 < \gamma < 1$, whereas $\epsilon^{\gamma} = 1$ for arbitrarily small ϵ when $\gamma = 0$.

The Gierer-Meinhardt model, being a dynamic system, implies the existence of equilibrium points. An equilibrium point in our context denotes a point where the partial derivatives of a and h with respect to time and position vanish. However, upon closer examination of the definition of the fractional derivative utilizing the Riemann-Liouville integral (2.41), we observe it vanishes solely when the differentiated function is zero. Consequently, we opt to employ a variant of the Riemann-Liouville integral expressed as

$$\frac{d^{\gamma} f(x)}{[d(x-c)]^{\gamma}} = \frac{-1}{\Gamma(-\gamma)} \int_{c}^{x} \frac{f(x) - f(x-\xi)}{\xi^{\gamma+1}} d\xi, \quad 0 < \gamma < 1.$$

For $c = 0$, and $x = t$ we have

$$\partial_t^{\gamma} f(t) = \frac{d^{\gamma} f(t)}{dt^{\gamma}} = \frac{-1}{\Gamma(-\gamma)} \int_{0}^{t} \frac{f(t) - f(t-\xi)}{\xi^{\gamma+1}} d\xi, \quad 0 < \gamma < 1. \tag{3.3}$$

3.1.1 Neumann Boundaries Conditions

As previously discussed, the interaction between activator and inhibitor molecules gives rise to distinctive spike patterns. Since our study revolves around a one-dimensional domain, these spikes propagate in both directions along the line until equilibrium is reached. For the purpose of our investigation, we have opted to focus on the symmetric interval $[-1, 1]$ as our chosen study domain. Neumann boundary conditions represent a fundamental type of boundary condition extensively employed in mathematical and physical models. They provide a framework for understanding how a given quantity evolves or interacts with its surroundings at the boundaries of a specified domain. In the context of the sub-diffusion reaction under examination, the Neumann boundary conditions play a crucial role by articulating how the rate of change in concentration (or flux) for both activators and inhibitors becomes null at $x = \pm 1$. This insight sheds light on the stability of the reaction at these specific points, preventing the entrance of any molecules into the study domain.

$$\partial_t^{\gamma} a = \epsilon^{2\gamma} a_{xx} - a + \frac{a^p}{h^q} \quad -1 < x < 1, \quad t > 0. \tag{3.4a}$$

$$\tau \partial_t^{\gamma} h = D h_{xx} - h + \epsilon^{-\gamma} \frac{a^m}{h^s} \quad -1 < x < 1, \quad t > 0. \tag{3.4b}$$

$$a_x(\pm 1, t) = h_x(\pm 1, t) = 0, \quad a(x, 0) = a_0(x), \quad h(x, 0) = h_0(x). \tag{3.4c}$$

with $t = 0$ representing the beginning of the reaction.

3.1.2 Asymptotic Solution of the Gierer-Meinhardt Model

An earlier analysis of the system composed of equations (1.1), (1.2), and (1.3) from [5] unveiled the existence of a solution (a, h) as ϵ approaches zero. This seminal study showed that the concentration a nullifies across the entire range of the problem, except at a finite set of points x_i, where i ranges from 1 to n. A time scale $\sigma = \epsilon^{\alpha} t$ allows to establish a local region around each x_i, where the concentration of the activator does not vanish. As a result, the behaviour of the solution function a can be captured separately within the inner and outer regions. A popular method for constructing these specific types of solutions that differ in nature from one region to another is called the "matched asymptotic expansions".

Matched asymptotic expansion

In mathematics, the technique known as matched asymptotic expansions is a common approach for deriving an approximation to the solution of an equation or a system of equations. This method involves the discovery of multiple distinct approximate solutions, each valid for a specific segment within the range of the independent variable. In each segment, the solution is approximated by an asymptotic series. Subsequently, these distinct solutions are combined to formulate a unique approximated solution, applicable across the entirety of the independent variable's value range. In the case of the Gierer-Meinhardt model the solution (a, h) is to be found separately in the outer and inner regions and matched. Upon examination of equation (3.4a), the presence of the parameter $\epsilon \to 0$ preceding the highest derivative a_{xx} and the reaction term $\frac{a^m}{h^s}$ in (3.4b) can be noticed. This scenario presents us with what is commonly referred to as a "singular perturbation problem". The application of the matched asymptotic expansions is still possible and has been successfully done when the time derivatives in system (3.2) were integer [5]. Hereinafter we will follow [6] in order to construct such a solution in the fractional case.

Perturbation theory

This section aims to provide valuable information about perturbation theory and is based on [9].

Perturbation methods: Perturbation methods are methods which rely on there being a dimensionless parameter ϵ in the problem that is small: $\|\epsilon\| \ll 1$.

Regular perturbation expansions The Taylor formula is one of the most known series expansions and is surely familiar to all of us: for an analytic function $f(x)$, we can expand close to a point $x = a$ as:

$$f(a+\epsilon) = f(a) + \epsilon f'(a) + \frac{1}{2}\epsilon^2 f''(a) + \cdots$$

However, for general functions $f(x)$ there are many ways this expansion can fail, including lack of convergence of the series, or simply an inability of the series to capture the behaviour of the function in a reasonable number of terms, after which the series is truncated; but the paradigm of the expansion in which a small change to x entails a small change to $f(x)$ is a powerful one, and the basis of singular perturbation expansions.
The basic principle of perturbation expansions is as follows. Given a problem, algebraic or differential, for a quantity f with independent variables $(t, x_1, x_2, ...)$ and a parameter ϵ, follow these steps.

(a) Set $\epsilon = 0$ and solve the resulting system (solution f_0 for definiteness).

(b) Perturb the system by allowing ϵ to be nonzero (but small in some sense).

(c) Formulate the solution to the new, perturbed system as a series.

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \cdots$$

(d) Expand the governing equations as a series in ϵ, collecting terms with equal powers of ϵ; solve them in turn as far as the solution is required.

Depending on where ϵ appears in the problem, it might be considered regular or singular. An example of a singular problem is, for instance, where ϵ multiplies the highest derivative of a differential equation or appears in the denominator in some expressions.

Dynamics of quasi-equilibrium patterns

As mentioned earlier, when we approach the limit $\epsilon \to 0$ in equation (3.4a), a solution is constructed. The activator's concentration becomes negligible across most of the domain, with notable increases occurring at specific points. However, upon closer examination, we find that these seemingly sudden jumps are, in fact, gradual. By scaling both time, from t to $\sigma = \epsilon^\alpha t$ and x to $y_i = \dfrac{x - x_i(\sigma)}{\epsilon^\gamma}$, we observe that the concentration gradually rises until reaching its peak at $x = x_i$. This phenomenon can be likened to someone traveling from Vancouver to Kamloops. Initially, they use a map of the entire province to navigate highways and cities. But upon arriving in Kamloops, they switch to a more detailed map specific to the town's neighborhoods and streets. The BC map corresponds to the original space and time scale (x, t) while the Kamloops map represents the new one (y_i, σ).

Concentration of the activator and the inhibitor in the inner region

Let us define by A and H to be the concentrations of the activator and inhibitor in the inner region. Applying singular perturbation expansions on A and H , we obtain for each y_i

$$A(y_i,\sigma) = a(x_i+\epsilon^{\gamma}y_i,\epsilon^{-\alpha}\sigma) = A_i^{(0)}(y_i,\sigma)+\epsilon^{\gamma}A_i^{(1)}(y_i,\sigma)+\epsilon^{2\gamma}A_i^{(2)}(y_i,\sigma)+\cdots \tag{3.5a}$$

$$H(y_i,\sigma) = h(x_i+\epsilon^{\gamma}y_i,\epsilon^{-\alpha}\sigma) = H_i^{(0)}(y_i,\sigma)+\epsilon^{\gamma}H_i^{(1)}(y_i,\sigma)+\epsilon^{2\gamma}H_i^{(2)}(y_i,\sigma)+\cdots \tag{3.5b}$$

Substituting (3.5a) in (3.4a) we obtain

$$\begin{aligned}\epsilon^{\alpha\gamma}\partial_\sigma^\gamma\left(A_i^{(0)}+\epsilon^\gamma A_i^{(1)}+\cdots\right) &= \epsilon^{2\gamma}\partial_x^2\left(A_i^{(0)}+\epsilon^\gamma A_i^{(1)}+\cdots\right)-\left(A_i^{(0)}+\epsilon^\gamma A_i^{(1)}+\cdots\right)\\ &\quad+\frac{\left(A_i^{(0)}+\epsilon^\gamma A_i^{(1)}+\cdots\right)^p}{\left(H_i^{(0)}+\epsilon^\gamma H_i^{(1)}+\cdots\right)^q}.\end{aligned} \tag{3.6}$$

We have

$$\partial_x^2 A_i = \partial_x^2 A_i(y_i) = \partial_x\left\{\epsilon^{-\gamma}\partial_{y_i}\left(A_i(y_i)\right)\right\} = \epsilon^{-2\gamma}\partial_{y_i}^2 A_i(y_i).$$

Applying that result to equation (3.6) we obtain

$$\begin{gathered}\epsilon^{\alpha\gamma}\partial_\sigma^\gamma\left(A_i^{(0)}+\epsilon^\gamma A_i^{(1)}+\cdots\right)=\\ \partial_{y_i}^2\left(A_i^{(0)}+\epsilon^\gamma A_i^{(1)}+\cdots\right)-\left(A_i^{(0)}+\epsilon^\gamma A_i^{(1)}+\cdots\right)+\frac{\left(A_i^{(0)}+\epsilon^\gamma A_i^{(1)}+\cdots\right)^p}{\left(H_i^{(0)}+\epsilon^\gamma H_i^{(1)}+\cdots\right)^q}.\end{gathered}$$

Subsequently,

$$\begin{aligned}\frac{\left(A_i^{(0)}+\epsilon^\gamma A_i^{(1)}+\cdots\right)^p}{\left(H_i^{(0)}+\epsilon^\gamma H_i^{(1)}+\cdots\right)^q} &= \frac{A_i^{(0)p}}{H_i^{(0)q}}\frac{\left(1+\epsilon^\gamma\dfrac{A_i^{(1)}}{A_i^{(0)}}+\cdots\right)^p}{\left(1+\epsilon^\gamma\dfrac{H_i^{(1)}}{H_i^{(0)}}+\cdots\right)^q}\\ &= \frac{A_i^{(0)p}}{H_i^{(0)q}}\left(1+\epsilon^\gamma\frac{A_i^{(1)}}{A_i^{(0)}}+\cdots\right)^p\left(1+\epsilon^\gamma\frac{H_i^{(1)}}{H_i^{(0)}}+\cdots\right)^{-q}.\end{aligned}$$

Additionally,

$$\left(1+\epsilon^{\gamma}\frac{A_i^{(1)}}{A_i^{(0)}}+\cdots\right)^p=(1+\xi_1)^p\sim(1+p\xi_1)=\left(1+p\Big(\epsilon^{\gamma}\frac{A_i^{(1)}}{A_i^{(0)}}+\cdots\Big)\right),$$

with $\xi_1=\Big(\epsilon^{\gamma}\frac{A_i^{(1)}}{A_i^{(0)}}+\cdots\Big)$.
Similarly, we have

$$\left(1+\epsilon^{\gamma}\frac{H_i^{(1)}}{H_i^{(0)}}+\cdots\right)^{-q}=(1+\xi_2)^{-q}\sim(1-q\xi_2)=\left(1-q\Big(\epsilon^{\gamma}\frac{H_i^{(1)}}{H_i^{(0)}}+\cdots\Big)\right),$$

with $\xi_2=\Big(\epsilon^{\gamma}\frac{H_i^{(1)}}{H_i^{(0)}}+\cdots\Big)$. Thus,

$$\begin{aligned}\frac{\Big(A_i^{(0)}+\epsilon^{\gamma}A_i^{(1)}+\cdots\Big)^p}{\Big(H_i^{(0)}+\epsilon^{\gamma}H_i^{(1)}+\cdots\Big)^q}&=\frac{A_i^{(0)^p}}{H_i^{(0)^q}}\left(1+p\Big(\epsilon^{\gamma}\frac{A_i^{(1)}}{A_i^{(0)}}+\cdots\Big)\right)\left(1-q\Big(\epsilon^{\gamma}\frac{H_i^{(1)}}{H_i^{(0)}}+\cdots\Big)\right)\\&=\frac{A_i^{(0)^p}}{H_i^{(0)^q}}\left(1-q\epsilon^{\gamma}\frac{H_i^{(1)}}{H_i^{(0)}}+\cdots+p\epsilon^{\gamma}\frac{A_i^{(1)}}{A_i^{(0)}}-pq\epsilon^{2\gamma}\frac{A_i^{(1)}}{A_i^{(0)}}\frac{H_i^{(1)}}{H_i^{(0)}}+\cdots\right).\end{aligned}$$

Upon truncating the equation at order $\mathcal{O}(\epsilon^{2\gamma})$ we obtain

$$\begin{aligned}\epsilon^{\alpha\gamma}\partial_{\sigma}^{\gamma}\left(A_i^{(0)}+\epsilon^{\gamma}A_i^{(1)}\right)\sim\partial_{y_i}^2\left(A_i^{(0)}+\epsilon^{\gamma}A_i^{(1)}\right)-\left(A_i^{(0)}+\epsilon^{\gamma}A_i^{(1)}\right)\\+\frac{A_i^{(0)^p}}{H_i^{(0)^q}}\left(1-q\epsilon^{\gamma}\frac{H_i^{(1)}}{H_i^{(0)}}+p\epsilon^{\gamma}\frac{A_i^{(1)}}{A_i^{(0)}}\right).\end{aligned}\tag{3.7}$$

Following the same process, and upon substituting (3.5b) in (3.4b) we obtain

$$\begin{aligned}\tau\epsilon^{\alpha\gamma}\partial_{\sigma}^{\gamma}\left(H_i^{(0)}+\epsilon^{\gamma}H_i^{(1)}\right)\sim\epsilon^{-2\gamma}D\partial_{y_i}^2\left(H_i^{(0)}+\epsilon^{\gamma}H_i^{(1)}\right)-\left(H_i^{(0)}+\epsilon^{\gamma}H_i^{(1)}\right)\\+\epsilon^{-\gamma}\frac{A_i^{(0)^m}}{H_i^{(0)^s}}\left\{1+\epsilon^{\gamma}\left(m\frac{A_i^{(1)}}{A_i^{(0)}}-s\frac{H_i^{(1)}}{H_i^{(0)^s}}\right)\right\}.\end{aligned}\tag{3.8}$$

Grouping terms of same magnitude in an asymptotic expansion

The method of truncation we recently employed in equations (3.7) and (3.8) is a technique used in mathematics to simplify complex functions or equations by focusing on their dominant behavior as variables approach certain limits. It involves breaking down a complex mathematical expression into its constituent terms and organizing them based on their relative orders of magnitude, as a variable approaches a certain limit, often denoted as a small parameter ϵ. The goal is to identify which terms dominate as ϵ approaches the limit and which terms become negligible. In our particular scenario, terms in equation (3.7) are grouped by order $\mathcal{O}(1)$ and $\mathcal{O}(\epsilon^{\gamma})$ representing respectively the equilibrium state and the drift. Similarly, terms in equation (3.8) are grouped by order $\mathcal{O}(\epsilon^{-2\gamma})$ and $\mathcal{O}(\epsilon^{-\gamma})$. This allows for an accurate approximation of a and h and captures the essential characteristics of the original equations while shedding unnecessary complexity. As we mentioned previously, the main objective of using perturbation expansions is to group terms of the same order into equations that are comparatively simpler and which satisfiy specific conditions. Since equations (3.7) and (3.8) depend on the α and τ parameters, a judicious choice of their magnitudes would greatly facilitate the resolution of these equations.

On one hand, let us suppose $\alpha < \gamma + 1$, for example $\alpha = \gamma + 1 - k$ with k a real number. We obtain

$$\begin{aligned}\epsilon^{\gamma^2-k\gamma+\gamma}\partial_\sigma^\gamma A_i^{(0)} + \epsilon^{\gamma^2-k\gamma+2\gamma}\partial_\sigma^\gamma A_i^{(1)} &\sim \partial_{y_i}^2(A_i^{(0)} + \epsilon^\gamma A_i^{(1)}) - (A_i^{(0)} + \epsilon^\gamma A_i^{(1)}) \\ &\quad + \frac{A_i^{(0)^p}}{H_i^{(0)^q}}\left(1 - q\epsilon^\gamma \frac{H_i^{(1)}}{H_i^{(0)}} + p\epsilon^\gamma \frac{A_i^{(1)}}{A_i^{(0)}}\right).\end{aligned}$$

From equation (3.33) in section(3.1.3), $\partial_\sigma^\gamma A_i \sim \mathcal{O}(\epsilon^{-\gamma^2})$. The previous expression is composed of terms of order $\mathcal{O}(\epsilon^{-k\gamma+\gamma})$, $\mathcal{O}(\epsilon^{-k\gamma+2\gamma})$, $\mathcal{O}(1)$, $\mathcal{O}(\epsilon^\gamma)$, and $\mathcal{O}(\epsilon^{2\gamma})$. By collecting terms of order $\mathcal{O}(\epsilon^{-k\gamma+\gamma})$ we obtain

$$\partial_\sigma^\gamma A_i^{(0)}(\sigma) = 0,$$

which is contradictory because $A_i^{(0)}$ is not constant.

On the other hand, for $\alpha > \gamma + 1$, such as $\alpha = \gamma + 1 + k$ we obtain

$$\begin{aligned}\epsilon^{\gamma^2+k\gamma+\gamma}\partial_\sigma^\gamma A_i^{(0)} + \epsilon^{\gamma^2+k\gamma+2\gamma}\partial_\sigma^\gamma A_i^{(1)} &\sim \partial_{y_i}^2(A_i^{(0)} + \epsilon^\gamma A_i^{(1)}) - (A_i^{(0)} + \epsilon^\gamma A_i^{(1)}) \\ &\quad + \frac{A_i^{(0)^p}}{H_i^{(0)^q}}\left(1 - q\epsilon^\gamma \frac{H_i^{(1)}}{H_i^{(0)}} + p\epsilon^\gamma \frac{A_i^{(1)}}{A_i^{(0)}}\right).\end{aligned}$$

By collecting terms of order $\mathcal{O}(1)$ and $\mathcal{O}(\epsilon^\gamma)$, we respectively obtain

$$\partial_{y_i}^2 A_i^{(0)} - A_i^{(0)} + \frac{A_i^{(0)^p}}{H_i^{(0)^q}} = 0. \tag{3.9}$$

$$\partial_{y_i}^2 A_i^{(1)} - A_i^{(1)} + \frac{A_i^{(0)^p}}{H_i^{(0)^q}}\left(p\frac{A_i^{(1)}}{A_i^{(0)^p}} - q\frac{H_i^{(1)}}{H_i^{(0)^q}}\right) = 0. \tag{3.10}$$

The system composed of equations (3.9) and (3.10) does not make sense because the former equation represents the stationary state condition, while the latter one of next order is intended to be time-dependent, illustrating the change in activator concentration over time, often referred as "drift". Since neither $\alpha > \gamma + 1$ nor $\alpha < \gamma + 1$ work, α needs to be $\gamma + 1$.

Solving order $\mathcal{O}(1)$ problem: For $\alpha = \gamma + 1$, and upon collecting terms of order $\mathcal{O}(1)$and $\mathcal{O}(\epsilon^{-2\gamma})$ in equations (3.7) and (3.8) respectively, we obtain

$$\partial^2_{y_i} A_i^{(0)}(y_i) - A_i^{(0)} + \frac{A_i^{(0)^p}}{H_i^{(0)^q}} = 0, \tag{3.11a}$$

$$\partial^2_{y_i} H_i^{(0)} = 0, \quad -\infty < y < \infty. \tag{3.11b}$$

From (3.11b), we have

$$\partial^2_{y_i} H_i^{(0)}(y_i, \sigma) = 0 \Rightarrow H_i^{(0)}(y_i, \sigma) = c_1(\sigma) y_i + c_2(\sigma),$$

with $c_1(\sigma)$, and $c_2(\sigma)$, functions to be determined. At infinity, $H_i^{(0)}$ is finite which imposes c_1 to be zero and $H_i^{(0)}(y_i, \sigma)$ to be y_i independent. $\bar{H}_i(\sigma)$ will then be used in place of $H_i^{(0)}(y_i, \sigma)$ throughout the rest of the document to express the independence from y_i. Finally, in order to simplify the denominator of the last term in equation (3.11a), we scale $A_i^{(0)}$ with a power of $\bar{H}_i$. We then set

$$A_i^{(0)}(\sigma) = \bar{H}_i^{\mathrm{B}}(\sigma) u(y_i),$$

with B and u to be determined.
By substituting $A_i^{(0)}$ into (3.11a), we obtain

$$\bar{H}_i^{\mathrm{B}} \partial^2_{y_i} u - \bar{H}_i^{\mathrm{B}} u + \frac{\bar{H}_i^{\mathrm{B}\,p}}{\bar{H}_i^q} u^p = 0,$$

$$\bar{H}_i^{\mathrm{B}} \left(\partial^2_{y_i} u - u + \bar{H}_i^{\mathrm{B}\,p-q-\mathrm{B}} u^p \right) = 0.$$

Subsequently,

$$\bar{H}_i^{\mathrm{B}} = 0 \quad \text{or} \quad \partial^2_{y_i} u - u + \bar{H}_i^{\mathrm{B}\,p-q-\mathrm{B}} u^p = 0.$$

Since $\bar{H}_i^{\mathrm{B}} \neq 0$, we get

$$\partial_{y_i}^2 u - u + \bar{H}_i^{\mathrm{B}\,p-q-\mathrm{B}} u^p = 0.$$

In order to get rid of the term $\bar{H}^{\mathrm{B}\,p-q-\mathrm{B}}$ and remain with a second order nonlinear differential equation, we set

$$\bar{H}_i^{\mathrm{B}\,p-q-\mathrm{B}} = 1 \Rightarrow \mathrm{B}\,p - q - \mathrm{B} = 0 \Rightarrow \mathrm{B} = \frac{q}{p-1}.$$

We finally obtain the equation

$$\frac{d^2u}{dy_i^2} - u + u^p = 0. \tag{3.12}$$

Homoclinic Solution: In mathematics and dynamics, a homoclinic solution is a curve that connects different equilibrium states within a system. This path, often represented as u, starts at one equilibrium state (in our case 0) and returns at the same equilibrium state. It is essentially a self-referential route that shows how a system settles at the same equilibrium state. To contrast, a 'heteroclinic solution' would connect two different equilibrium states in the system. The homoclinic solution is given by

$$u(y) = \left(\frac{p+1}{2}\operatorname{sech}^2\frac{(p-1)y}{2}\right)^{\dfrac{1}{p-1}}.$$

It is the unique solution of the following boundary value problem

$$u'' - u + u^p = 0, \quad -\infty < y < \infty, \tag{3.13a}$$

$$u'(0) = 0, \quad u(0) > 0, \quad \text{and} \quad \lim_{|y|\to\infty} u = 0. \tag{3.13b}$$

Solving order $\mathcal{O}(\epsilon^\gamma)$ problem: Upon collecting terms of order $\mathcal{O}(\epsilon^\gamma)$ and $\mathcal{O}(\epsilon^{-\gamma})$ in equations (3.7) and (3.8), we have

$$\epsilon^{\alpha\gamma-\gamma}\partial_\sigma^\gamma A_i^{(0)} = \partial_{y_i}^2 A_i^{(1)} - A_i^{(1)} + \frac{A_i^{(0)^p}}{\bar{H}_i^q}\left(p\frac{A_i^{(1)}}{A_i^{(0)}} - q\frac{H_i^{(1)}}{\bar{H}_i}\right), \tag{3.14a}$$

$$D\partial_{y_i}^2 H_i^{(1)}(y_i(\sigma)) = -\frac{A_i^{(0)^m}}{\bar{H}_i^s}. \tag{3.14b}$$

Substituting $A_i^{(0)} = \bar{H}_i^{\mathrm{B}}(\sigma)u(y_i)$ in both equations (3.14a) and (3.14b) leads to

$$\epsilon^{\gamma^2}\partial_\sigma^\gamma(\bar{H}_i^{\mathrm{B}}u) = \partial_{y_i}^2 A_i^{(1)} - A_i^{(1)} + \frac{A_i^{(0)p}}{\bar{H}_i^q} p \frac{A_i^{(1)}}{A_i^{(0)}} - \frac{A_i^{(0)p}}{\bar{H}_i^q} q \frac{H_i^{(1)}}{\bar{H}_i},$$

$$D\partial_{y_i}^2 H_i^{(1)} = -H^{\mathrm{B}\,m-s}u^m.$$

Subsequently,

$$\epsilon^{\gamma^2}\partial_\sigma^\gamma(\bar{H}_i^{\mathrm{B}}u) = \partial_{y_i}^2 A_i^{(1)} - A_i^{(1)} + pA_i^{(1)}\bar{H}_i^{\mathrm{B}(p-1)-q}u^{p-1} - q\frac{H_i^{(1)}}{\overline{H}_i}\overline{H}_i^{\mathrm{B}\,p-q}u^p,$$

$$D\partial_{y_i}^2 H_i^{(1)} = -H_i^{\mathrm{B}\,m-s}u^m.$$

Since $\mathrm{B}\,p - \mathrm{B}\,-q = 0$, $\partial_\sigma^\gamma u \sim -\epsilon^{-\gamma^2}\,\mathrm{sign}\left(\frac{dx_i}{d\sigma}\right)\left|\frac{dx_i}{d\sigma}\right|^\gamma \mathcal{D}_{y_i}^\gamma u$ and $\mathcal{L}_0 = \frac{d^2}{dy_i^2} - 1 + pu^{p-1}$ a linear operator in lemma (2.2) from [6], we finally obtain

$$\mathcal{L}_0 A_i^{(1)} = \left(q\frac{H_i^{(1)}}{\overline{H}_i}u^p - \mathrm{sign}\left(\frac{dx_i}{d\sigma}\right)\left|\frac{dx_i}{d\sigma}\right|^\gamma \mathcal{D}_{y_i}^\gamma u\right)\overline{H_i}^{\mathrm{B}}, \tag{3.15a}$$

$$D\partial_{y_i}^2 H_i^{(1)} = -\bar{H}_i^{\mathrm{B}\,m-s}u^m. \tag{3.15b}$$

Note:

$$\mathcal{D}_t^\gamma u(t) = \mathrm{sign}\left(\frac{dx_i}{d\sigma}\right)\frac{1}{\Gamma(-\gamma)}\int_0^\infty \left\{u(t) - u\left(t + \mathrm{sign}\left(\frac{dx_i}{d\sigma}\right)y\right)\right\}\left(\frac{1}{y}\right)^{\gamma+1} dy.$$

The fractional operator $\mathcal{D}_{y_i}^\gamma$ can be regarded as the left or right propagating fractional derivative according to whether $\frac{dx_i}{d\sigma}$ is positive or negative, and will be study in more details in section 4.1.

Equation (3.15a) is of the form $f(a) = b$ with f being a linear operator and a and b common functions. In order to find a in the previous example, we have two options. In the case where f is invertible, we have $a = f^{-1}(b)$, which is not possible in this case because $\ker \mathcal{L}_0 = \frac{du}{dy_i} \neq \emptyset$. Otherwise, the Fredholm alternative stipulates that a can be found if $\ker f$ is orthogonal to b with a and b integrable functions. This condition implies that $< \ker f, b >= 0$ which leads to

$$\left\langle \frac{du}{dy_i}, \left(q\frac{H_i^{(1)}}{\overline{H}_i}u^p - \mathrm{sign}\left(\frac{dx_i}{d\sigma}\right)\left|\frac{dx_i}{d\sigma}\right|^\gamma \mathcal{D}_{y_i}^\gamma u\right)\overline{H_i}^{\mathrm{B}}\right\rangle = 0.$$

We then obtain the solvability condition

$$\int_{-\infty}^{\infty} \frac{du}{dy_i} \left(q \frac{H_i^{(1)}}{\overline{H_i}} u^p - \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \left|\frac{dx_i}{d\sigma}\right|^{\gamma} \mathcal{D}_{y_i}^{\gamma} u \right) \overline{H_i}^{\mathrm{B}} dy_i = 0.$$

Subsequently,

$$\int_{-\infty}^{\infty} \frac{du}{dy_i} q \frac{H_i^{(1)}}{\overline{H_i}} u^p \; dy_i - \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \left|\frac{dx_i}{d\sigma}\right|^{\gamma} \int_{-\infty}^{\infty} \frac{du}{dy_i} \mathcal{D}_{y_i}^{\gamma} u \; dy_i = 0. \tag{3.16}$$

By integrating by parts the first term of equation (3.16), we obtain

$$\frac{q}{\overline{H_i}(p+1)} \left(H_i^{(1)} u^{p+1} \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \partial_{y_i} H_i^{(1)} u^{p+1} dy_i \right) - \\ \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \left|\frac{dx_i}{d\sigma}\right|^{\gamma} \int_{-\infty}^{\infty} \frac{du}{dy_i} \mathcal{D}_{y_i}^{\gamma} u \; dy_i = 0.$$

Subsequently, since u decays exponentially at the boundaries we obtain

$$-\frac{q}{\overline{H_i}(p+1)} \int_{-\infty}^{\infty} \partial_{y_i} H_i^{(1)} u^{p+1} dy_i - \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \left|\frac{dx_i}{d\sigma}\right|^{\gamma} \int_{-\infty}^{\infty} \frac{du}{dy_i} \mathcal{D}_{y_i}^{\gamma} u \; dy_i = 0.$$

By performing a second integration by parts on the first term, we have

$$-\frac{q}{\overline{H_i}(p+1)} \left(\partial_{y_i} H_i^{(1)} \int_0^{y_i} u^{p+1}(t) dt \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \partial_{y_i}^2 H_i^{(1)} \left(\int_0^{y_i} u^{p+1}(t) dt \right) dy_i \right) - \\ \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \left|\frac{dx_i}{d\sigma}\right|^{\gamma} \int_{-\infty}^{\infty} \frac{du}{dy_i} \mathcal{D}_{y_i}^{\gamma} u \; dy_i = 0.$$

Since u is even, it implies that u^{p+1} is also even and $\int_0^{y_i} u^{p+1}(t)dt$ is odd. Also, from (3.15b) we have $\partial_{y_i}^2 H_i^{(1)}$ even, thus $\partial_{y_i}^2 H_i^{(1)} \left(\int_0^{\infty} u^{p+1}(t) \right) dt$ is odd and finally $\int_{-\infty}^{\infty} \partial_{y_i}^2 H_i^{(1)} \left(\int_0^{\infty} u^{p+1}(t) dt \right) dy_i = 0$. We then obtain

$$-\frac{q}{\overline{H_i}(p+1)} \left(\int_0^{\infty} u^{p+1} dy_i \lim_{y_i \to \infty} \partial_{y_i} H_i^{(1)} - \int_0^{-\infty} u^{p+1} dy_i \lim_{y_i \to -\infty} \partial_{y_i} H_i^{(1)} \right) \\ - \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \left|\frac{dx_i}{d\sigma}\right|^{\gamma} \int_{-\infty}^{\infty} \frac{du}{dy_i} \mathcal{D}_{y_i}^{\gamma} u \; dy_i = 0.$$

Subsequently,

$$-\frac{q}{\overline{H_i}(p+1)} \left(\int_0^{\infty} u^{p+1} dy_i \lim_{y_i \to \infty} \partial_{y_i} H_i^{(1)} + \int_0^{\infty} u^{p+1} dy_i \lim_{y_i \to -\infty} \partial_{y_i} H_i^{(1)} \right) - \\ \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \left|\frac{dx_i}{d\sigma}\right|^{\gamma} \int_{-\infty}^{\infty} \frac{du}{dy_i} \mathcal{D}_{y_i}^{\gamma} u \; dy_i = 0.$$

Then,

$$-\frac{q}{2\overline{H_i}(p+1)}\int_{-\infty}^{\infty}u^{p+1}dy_i\left(\lim_{y_i\to\infty}\partial_{y_i}H_i^{(1)}+\lim_{y_i\to-\infty}\partial_{y_i}H_i^{(1)}\right)-$$
$$\operatorname{sign}\left(\frac{dx_i}{d\sigma}\right)\left|\frac{dx_i}{d\sigma}\right|^{\gamma}\int_{-\infty}^{\infty}\frac{du}{dy_i}\mathcal{D}_{y_i}^{\gamma}u\ dy_i=0,$$

and finally

$$\begin{aligned}&\frac{q}{2\overline{H_i}(p+1)}\int_{-\infty}^{\infty}u^{p+1}dy_i\left(\lim_{y_i\to\infty}\partial_{y_i}H_i^{(1)}+\lim_{y_i\to-\infty}\partial_{y_i}H_i^{(1)}\right)\\&=-\operatorname{sign}\left(\frac{dx_i}{d\sigma}\right)\left|\frac{dx_i}{d\sigma}\right|^{\gamma}\int_{-\infty}^{\infty}\frac{du}{dy_i}\mathcal{D}_{y_i}^{\gamma}u\ dy_i\end{aligned}. \tag{3.17}$$

Concentration of the activator and the inhibitor in the outer region

Let a and h denote respectively the concentrations of the activator and the inhibitor in the outer region.The concentration of the activator is null in the outer region except at the limits. Therefore, our focus is on studying the concentration of the inhibitor in the outer region and the limits. Similar to the inner region, applying the singular perturbation expansions on h leads to

$$h(x,t)=h^{(0)}(x,\sigma)+\epsilon^{\gamma}h^{(1)}(x,\sigma)+\mathcal{O}(\epsilon^{2\gamma}). \tag{3.18}$$

As previously mentioned, we have $y_i=\dfrac{x-x_i}{\epsilon^{\gamma}}$ with $i=1,\cdots,n$. This implies that the domain contains n positions x_i where the concentration of the activator is not null. If we returned to equation (3.4b) of the model, the nonlinear function or term $\epsilon^{-\gamma}\dfrac{a^m(x,t)}{h^s(x,t)}$ has the following characteristics:

- $\epsilon^{-\gamma}\dfrac{a^m(x,t)}{h^s(x,t)}$ is obtained by collecting and summing its values around each position x_i.
- $\epsilon^{-\gamma}\dfrac{a^m(x,t)}{h^s(x,t)}$ vanishes on the entire outer domain as a also vanishes there.
- Since a vanishes everywhere except around $x=x_i$, and h is independent of x in the same region, we have

$$\epsilon^{-\gamma}\frac{a^m(x,t)}{h^s(x,t)}\sim\epsilon^{-\gamma}\frac{A^{(0)^m}}{H^{(0)^s}}=\epsilon^{-\gamma}\bar{H}_i^{\mathrm{B}\,m-s}u^m,$$

then

$$\int_{x_i^-}^{x_i^+}\epsilon^{-\gamma}\frac{a^m(x,t)}{h^s(x,t)}dx\sim\int_{-\infty}^{\infty}\frac{A_i^{(0)^m}}{\bar{H}_i^s}dy_i=\bar{H}_i^{\mathrm{B}\,m-s}\int_{-\infty}^{\infty}u^m dy_i=\text{constant}.$$

Due to these localised behaviors, $\epsilon^{-\gamma}\dfrac{a^m(x,t)}{h^s(x,t)}$ can be expressed as a linear combination of the weighted Dirac δ functions:

$$\epsilon^{-\gamma}\frac{a^m(x,t)}{h^s(x,t)} \sim b_m \sum_{i=1}^{n} \bar{H}_i^{\mathrm{B}\,m-s}\delta(x-x_i), \tag{3.19}$$

with

$$b_m = \int_{-\infty}^{\infty} u^m dy_i = \frac{2}{p-1}\left(\frac{p+1}{2}\right)^{\dfrac{m}{p-1}} \frac{\Gamma(\frac{1}{2})\Gamma(\dfrac{m}{p-1})}{\Gamma(\dfrac{1}{2}+\dfrac{m}{p-1})},$$

as proved in section (3.1.3) and δ from [8, Page 64] defined as

$$\delta(t) = \begin{cases} 0 & \text{if} \quad t \neq 0 \\ \infty & \text{if} \quad t = 0 \end{cases} \qquad \text{and} \qquad \int_{-\infty}^{\infty} \delta(t)dt = 1.$$

For $t = x - x_i$ it can be rewritten as

$$\delta(x-x_i) = \begin{cases} 0 & \text{if} \quad x \neq x_i \\ \infty & \text{if} \quad x = x_i \end{cases}, \quad \text{and} \quad \int_{x_i^-}^{x_i^+} \delta(x-x_i)dx = 1.$$

Substituting (3.19) in (3.4b) leads to

$$\tau\epsilon^{\alpha\gamma}\partial_\sigma^\gamma h^{(0)}(\sigma) \sim Dh_{xx}^{(0)} - h^{(0)} + b_m \sum_{i=1}^{n} \bar{H}_i^{\mathrm{B}\,m-s}\delta(x-x_i).$$

Upon collecting terms of order $\mathcal{O}(1)$, we obtain

$$Dh_{xx}^{(0)} - h^{(0)} = -b_m \sum_{i=1}^{n} \bar{H}_i^{\mathrm{B}\,m-s}\delta(x-x_i). \tag{3.20}$$

The solution of (3.20) is expressed as

$$h^{(0)}(x,t) = b_m \sum_{i=1}^{n} \bar{H}_i^{\mathrm{B}\,m-s}G(x;x_i),$$

where the Green's function $G(x;x_i)$ satisfies the equation

$$DG_{xx} - G = -\delta(x-x_i), \quad -1 < x < 1, \tag{3.21a}$$

$$G_x(\pm 1; x_i) = 0. \tag{3.21b}$$

The perturbation expansions of h is expressed as

$$h(x,\sigma) \sim h^{(0)}(x,\sigma) + \epsilon^{\gamma} h^{(1)}(x,\sigma) + \mathcal{O}(\epsilon^{2\gamma}).$$

At infinity, we have

$$h^{(0)} = \bar{H}_i \quad \text{and} \quad h^{(1)} = H_i^{(1)}.$$

Upon matching the concentrations of the inhibitor in the inner and outer region, we obtain

$$\lim_{y_i \to \pm\infty} h = \lim_{y_i \to \pm\infty} \left(\bar{H}_i + \epsilon^{\gamma} H_i^{(1)} \right),$$

and then

$$\lim_{y_i \to \pm\infty} \frac{dH_i^{(1)}}{dy_i} = \lim_{y_i \to \pm\infty} \epsilon^{-\gamma} \frac{\partial}{\partial_{y_i}} \left(h(x_i + \epsilon^{\gamma} y_i, \sigma) - \bar{H}_i \right) = \lim_{x \to x_i^{\pm}} \frac{\partial h^{(0)}}{\partial_x}.$$

We then have

$$\lim_{y_i \to -\infty} \partial_{y_i} H_i^{(1)} = \lim_{x \to x_i^-} h_x^{(0)} = \lim_{x \to x_i^-} b_m \sum_{i=1}^{n} \bar{H}_i^{\mathrm{B}\, m-s} G_x(x; x_i).$$

Subsequently,

$$\lim_{y_i \to -\infty} \partial_{y_i} H_i^{(1)} = b_m \sum_{\substack{j=1 \\ j \neq i}}^{n} \bar{H}_i^{\mathrm{B}\, m-s} G_x(x; x_j) + b_m \bar{H}^{\mathrm{B}\, m-s} G_x(x_i^-; x_i).$$

Similarly,

$$\lim_{y_i \to \infty} \partial_{y_i} H_i^{(1)} = b_m \sum_{\substack{j=1 \\ j \neq i}}^{n} \bar{H}_i^{\mathrm{B}\, m-s} G_x(x; x_j) + b_m \bar{H}^{\mathrm{B}\, m-s} G_x(x_i^+; x_i).$$

Therefore, we have

$$\begin{aligned} \lim_{y_i \to -\infty} \partial_{y_i} H_i^{(1)} + \lim_{y_i \to \infty} \partial_{y_i} H_i^{(1)} &= 2b_m \sum_{\substack{j=1 \\ j \neq i}}^{n} \bar{H}_i^{\mathrm{B}\, m-s} G_x(x; x_j) \\ &\quad + b_m \left(\bar{H}^{\mathrm{B}\, m-s} G_x(x_i^-; x_i) + \bar{H}^{\mathrm{B}\, m-s} G_x(x_i^+; x_i) \right). \end{aligned}$$

Then,

$$\lim_{y_i \to -\infty} \partial_{y_i} H_i^{(1)} + \lim_{y_i \to \infty} \partial_{y_i} H_i^{(1)} = 2b_m \left(\sum_{\substack{j=1 \\ j \neq i}}^{n} \bar{H}_i^{\mathrm{B}\, m-s} G_x(x; x_j) + \bar{H}^{\mathrm{B}\, m-s} \langle G_x \rangle_i \right), \quad (3.22)$$

with

$$\langle G_x \rangle_i = \frac{1}{2}\Big(G_x^-(x_i^-; x_i) + G_x^+(x_i^+; x_i)\Big),$$

where G^+ and G^- are defined as

$$G^-(x; x_i) = \frac{w_0 \cosh(w_0 x_i - w_0)}{\sinh(2w_0)} \cosh(w_0 x + w_0), \quad -1 < x < x_i,$$

$$G^+(x; x_i) = \frac{w_0 \cosh(w_0 x_i + w_0)}{\sinh(2w_0)} \cosh(w_0 x - w_0), \quad x_i < x < 1,$$

from section 3.1.3 with $w_0 = D^{-\frac{1}{2}}$.

Upon substituting (3.22) in the solvability condition (3.17), we obtain

$$\frac{q}{2(p+1)\bar{H}_i} \int_{-\infty}^{\infty} u^{p+1} dy_i \left(2b_m \left(\sum_{\substack{j=1 \\ j \neq i}}^{n} \bar{H}_i^{\mathrm{B}\, m-s} G_x(x; x_j) + \bar{H}^{\mathrm{B}\, m-s} \langle G_x \rangle_i \right) \right)$$
$$= - \left| \frac{dx_i}{d\sigma} \right|^{\gamma} \operatorname{sign}\left(\frac{dx_i}{d\sigma} \right) \int_{-\infty}^{\infty} \frac{du}{dy_i} \mathcal{D}_{y_i}^{\gamma} u \; dy_i.$$

Subsequently,

$$- \left| \frac{dx_i}{d\sigma} \right|^{\gamma} \operatorname{sign}\left(\frac{dx_i}{d\sigma} \right) = \frac{q b_m}{(p+1)\bar{H}_i} \left(\sum_{\substack{j=1 \\ j \neq i}}^{n} \bar{H}_i^{\mathrm{B}\, m-s} G_x(x; x_j) + \bar{H}^{\mathrm{B}\, m-s} \langle G_x \rangle_i \right) \frac{\displaystyle\int_{-\infty}^{\infty} u^{p+1} dy_i}{\displaystyle\int_{-\infty}^{\infty} \frac{du}{dy_i} \mathcal{D}_{y_i}^{\gamma} u \; dy_i}.$$

We finally obtain the differential algerbraic system

$$- \left| \frac{dx_i}{d\sigma} \right|^{\gamma} \operatorname{sign}\left(\frac{dx_i}{d\sigma} \right) = \frac{q b_m}{(p+1)\bar{H}_i} \left(\sum_{\substack{j=1 \\ j \neq i}}^{n} \bar{H}_i^{\mathrm{B}\, m-s} G_x(x; x_j) + \bar{H}^{\mathrm{B}\, m-s} \langle G_x \rangle_i \right) f(p; y), \tag{3.23a}$$

$$\bar{H}_i(\sigma) = h^{(0)}(x,t) = b_m \sum_{i=1}^{n} \bar{H}_i^{\mathrm{B}\, m-s} G(x; x_i), \quad b_m = \int_{-\infty}^{\infty} u^m dy_i, \tag{3.23b}$$

$$f(p; y) = \left(\int_{-\infty}^{\infty} u^{p+1} dy_i \right) \Big/ \left(\int_{-\infty}^{\infty} \frac{du}{dy_i} \mathcal{D}_{y_i}^{\gamma} u dy_i \right). \tag{3.23c}$$

Note:

Section 3.1.3 provides proofs for certain results utilized in Chapter 3. If these have been previously reviewed, the reader should then proceed to Chapter 4.

3.1.3 Auxiliary Proofs

The following properties, along with their accompanying proofs, were frequently utilized to derive important results in this chapter:

A) We aim to show that $\partial_\sigma^\gamma A \sim \epsilon^{-\gamma^2}$, with A being the concentration of the activator in the inner region. Starting with the definition in equation (3.3), we have

$$\partial_\sigma^\gamma A(y_i(\sigma)) = -\frac{1}{\Gamma(-\gamma)} \int_0^\sigma \left(A(y_i(\sigma)) - A\Big(y_i(\sigma-\zeta)\Big) \right) \frac{d\zeta}{\zeta^{\gamma+1}}. \tag{3.24}$$

Next, let us introduce a new variable ξ defined as:

$$\xi = \epsilon^{-\gamma}\Big(x_i(\sigma-\zeta) - x_i(\sigma)\Big). \tag{3.25}$$

To find ζ in terms of ξ, when $\epsilon \ll 1$, we expand x_i as ($x_i \in C^\infty$):

$$x_i(\sigma-\zeta) - x_i(\sigma) = -\frac{dx_i}{d\sigma}\zeta + \frac{1}{2}\frac{d^2x_i}{d\sigma^2}\zeta^2 - + \cdots. \tag{3.26}$$

Substituting equation (3.26) into (3.25), we obtain

$$\xi = \epsilon^{-\gamma}\left(-\frac{dx_i}{d\sigma}\zeta + \frac{1}{2}\frac{d^2x_i}{d\sigma^2}\zeta^2 - + \cdots \right). \tag{3.27}$$

From Equation (3.27), we deduce

$$\zeta = -\left(\frac{dx_i}{d\sigma}\right)^{-1} \left(\epsilon^\gamma \xi - \frac{1}{2}\frac{d^2x_i}{d\sigma^2}\zeta^2 - + \cdots \right). \tag{3.28}$$

By a recursive substitution of ζ in (3.28), one obtains

$$\zeta = -\left(\frac{dx_i}{d\sigma}\right)^{-1} \left\{ \epsilon^\gamma \xi - \frac{1}{2}\frac{d^2x_i}{d\sigma^2} \left(-\left(\frac{dx_i}{d\sigma}\right)^{-1} \left(\epsilon^\gamma \xi - \frac{1}{2}\frac{d^2x_i}{d\sigma^2}\zeta^2 + \cdots - \cdots \right)\right)^2 \right\}. \tag{3.29}$$

Subsequently, we find

$$\zeta \sim -\epsilon^{\gamma} \left(\frac{dx_i}{d\sigma}\right)^{-1} \xi + \mathcal{O}(\epsilon^{2\gamma}). \tag{3.30}$$

Additionally, we have

$$\frac{x - x_i(\sigma - \xi)}{\epsilon^{\gamma}} = \frac{x - x_i(\sigma) + x_i(\sigma) - x_i(\sigma - \xi)}{\epsilon^{\gamma}} = y_i - \xi. \tag{3.31}$$

Upon substituting equations (3.30) and (3.29) into (3.24) and the value of ζ in equation (3.28), we obtain

$$\partial_{\sigma}^{\gamma} A(y_i(\sigma)) = -\frac{\epsilon^{-\gamma^2}}{\Gamma(-\gamma)} - \left(\frac{dx_i}{d\sigma}\right)^{-1} \int_0^{-\infty \mathrm{sign}(\frac{dx_i}{d\sigma})} \left\{ A(y_i(\sigma)) - A\Big(y_i(\sigma - \xi)\Big) \right\} \left(-\frac{dx_i}{d\sigma}\frac{1}{\xi}\right)^{\gamma+1} d\xi, \tag{3.32}$$

with the integrals boundaries obtained as follows.
We have $\zeta \sim -\epsilon^{\gamma} \left(\frac{dx_i}{d\sigma}\right)^{-1} \xi \Rightarrow d\zeta = \epsilon^{\gamma} \left(\frac{-dx_i}{d\sigma}\right)^{-1} d\xi.$
Moreover,

$$\xi \sim \epsilon^{-\gamma} \left(-\frac{dx_i}{d\sigma}\right) \zeta,$$

$$\zeta \to 0 \Rightarrow \xi \to 0, \quad \zeta \to \sigma \Rightarrow \xi \to \epsilon^{-\gamma} \left(-\frac{dx_i}{d\sigma}\right) \sigma,$$

$$\epsilon \to 0 \Rightarrow \xi \to -\operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \infty.$$

Let us rewrite $\partial_{\sigma}^{\gamma} A(y_i(\sigma))$ as

$$\partial_{\sigma}^{\gamma} A(y_i(\sigma)) \sim -\epsilon^{-\gamma^2} \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \left|\frac{dx_i}{d\sigma}\right|^{\gamma} \mathcal{D}_{y_i}^{\gamma} A(y_i), \tag{3.33}$$

with

$$\mathcal{D}_{y_i}^{\gamma} A(y_i) = \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \frac{1}{\Gamma(-\gamma)} \int_0^{\infty} \left\{ A(y_i) - A\left(y_i + \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right) \xi_1\right) \right\} \left(\frac{1}{\xi_1}\right)^{\gamma+1} d\xi_1. \tag{3.34}$$

$\mathcal{D}_{y_i}^{\gamma}$ can be regarded as the left or right propagating fractional derivative according to whether $\frac{dx_i}{d\sigma}$ is positive or negative.
We have

$$\partial_{\sigma}^{\gamma} A(y_i(\sigma)) = -\frac{\epsilon^{-\gamma^2}}{\Gamma(-\gamma)} \left(-\frac{dx_i}{d\sigma}\right)^{-1} \int_0^{-\infty\, \mathrm{sign}(\frac{dx_i}{d\sigma})} \left\{ A(y_i(\sigma)) - A\Big(y_i(\sigma - \xi)\Big) \right\} \left(-\frac{dx_i}{d\sigma}\frac{1}{\xi}\right)^{\gamma+1} d\xi.$$

Let us have $\xi = -\operatorname{sign}\left(\frac{dx_i}{d\sigma}\right)\xi_1$.

Firstly let us suppose $\frac{dx_i}{d\sigma} < 0$, then $\xi = \xi_1$, and $d\xi = d\xi_1$.

$$\begin{aligned} \xi \to 0 \quad &\Rightarrow \quad \xi_1 \to 0, \\ \xi \to \infty \quad &\Rightarrow \quad \xi_1 \to \infty. \end{aligned}$$

$$\begin{aligned} \partial_\sigma^\gamma A(y_i(\sigma)) &= -\frac{\epsilon^{-\gamma^2}}{\Gamma(-\gamma)} \left(-\frac{dx_i}{d\sigma}\right)^{-1} \int_0^\infty \left\{ A(y_i(\sigma)) - A\Big(y_i(\sigma - \xi_1)\Big) \right\} \left(-\frac{dx_i}{d\sigma}\frac{1}{\xi_1}\right)^{\gamma+1} d\xi_1 \\ &= -\frac{\epsilon^{-\gamma^2}}{\Gamma(-\gamma)} \left(-\frac{dx_i}{d\sigma}\right)^{\gamma} \int_0^\infty \left\{ A(y_i(\sigma)) - A\Big(y_i(\sigma - \xi_1)\Big) \right\} \frac{d\xi_1}{\xi_1^{\gamma+1}}. \end{aligned}$$

We have

$$\begin{aligned} -\frac{dx_i}{d\sigma} &= \left|-\frac{dx_i}{d\sigma}\right| \operatorname{sign}\left(-\frac{dx_i}{d\sigma}\right) = \left|\frac{dx_i}{d\sigma}\right|, \\ \left(-\frac{dx_i}{d\sigma}\right)^\gamma &= \left|\frac{dx_i}{d\sigma}\right|^\gamma. \end{aligned}$$

Then,

$$\partial_\sigma^\gamma A(y_i(\sigma)) = -\frac{\epsilon^{-\gamma^2}}{\Gamma(-\gamma)} \left|\frac{dx_i}{d\sigma}\right|^\gamma \int_0^\infty \left\{ A(y_i(\sigma)) - A\Big(y_i(\sigma - \xi_1)\Big) \right\} \frac{d\xi_1}{\xi_1^{\gamma+1}}. \tag{3.35}$$

Secondly, let us use suppose $\frac{dx_i}{d\sigma} > 0$, then $\xi = -\xi_1$, and $d\xi = -d\xi_1$.

$$\begin{aligned} \xi \to 0 \quad &\Rightarrow \quad \xi_1 \to 0, \\ \xi \to -\infty \quad &\Rightarrow \quad \xi_1 \to \infty. \end{aligned}$$

Subsequently,

$$\begin{aligned} \partial_\sigma^\gamma A(y_i(\sigma)) &= -\frac{\epsilon^{-\gamma^2}}{\Gamma(-\gamma)} \left(\frac{dx_i}{d\sigma}\right)^{-1} \int_0^\infty \left\{ A(y_i(\sigma)) - A\Big(y_i(\sigma + \xi_1)\Big) \right\} \left(\frac{dx_i}{d\sigma}\frac{1}{\xi_1}\right)^{\gamma+1} (-d\xi_1) \\ &= -\frac{\epsilon^{-\gamma^2}}{\Gamma(-\gamma)} \left(\frac{dx_i}{d\sigma}\right)^{\gamma} \int_0^\infty \left\{ A(y_i(\sigma)) - A\Big(y_i(\sigma + \xi_1)\Big) \right\} \left(\frac{1}{\xi_1}\right)^{\gamma+1} d\xi_1. \end{aligned}$$

Then,

$$\partial_\sigma^\gamma A(y_i(\sigma)) = -\frac{\epsilon^{-\gamma^2}}{\Gamma(-\gamma)} \left|\frac{dx_i}{d\sigma}\right|^\gamma \int_0^\infty \left\{ A(y_i(\sigma)) - A\Big(y_i(\sigma + \xi_1)\Big) \right\} \left(\frac{1}{\xi_1}\right)^{\gamma+1} d\xi_1. \tag{3.36}$$

Considering (3.35) and (3.36) , we obtain the general form (3.33).

B) Let us prove that $\dfrac{du}{dy}$ is the only element of $\ker \mathcal{L}_0$. Let us first prove that $\dfrac{du}{dy} \in \ker \mathcal{L}_0$ or $\quad \mathcal{L}_0 \dfrac{du}{dy} = 0.$

$$\mathcal{L}_0 \frac{du}{dy} = \frac{d^2}{dy^2}\left(\frac{du}{dy}\right) - \frac{du}{dy} + p\frac{du}{dy}u^{p-1} = \frac{d}{dy}\left(\frac{d^2u}{dy^2} - u + u^p\right) = \frac{d}{dy}\left(u'' - u + u^p\right) = 0.$$

Let's now demonstrate that $\dfrac{du}{dy}$ is the sole element of $\ker \mathcal{L}_0$. As a consequence of the Sturm-Liouville theory, it follows that for a specific eigenvalue problem $\mathcal{L}_0\psi = \nu\psi$, there exists a unique eigenfunction ψ associated with each eigenvalue ν. Furthermore, the number of zeros of the eigenfunction ψ is equal to the number of its corresponding eigenvalue within the entire set of eigenvalues minus one. In our specific case, we find $\mathcal{L}_0 u_1 = 0$, which can be expressed as $\mathcal{L}_0 u_1 = 0 \cdot u_1$, with u_1 an eigenfunction associated with the eigenvalue 0. Thus, u_1 represents the unique eigenfunction associated with the eigenvalue 0. This conclusion implies that $u_1 = \dfrac{du}{dy_i}$ is the only solution to the differential equation $\mathcal{L}_0 \dfrac{du}{dy_i} = 0$ and, consequently, the sole element within $\ker \mathcal{L}_0$.

C) Let us find $b_m = \displaystyle\int_{-\infty}^{\infty} u^m dy$, we have

$$\begin{aligned} b_m &= \int_{-\infty}^{\infty} u^m dy = \int_{-\infty}^{\infty} \left\{ \left(\frac{p+1}{2}\right) \operatorname{sech}^2\left(\frac{(p-1)}{2}y\right) \right\}^{\frac{m}{p-1}} dy \\ &= \int_{-\infty}^{\infty} \left(\frac{p+1}{2}\right)^{\frac{m}{p-1}} \operatorname{sech}^{\frac{2m}{p-1}}\left(\frac{(p-1)}{2}y\right) dy. \end{aligned}$$

For $\quad u = \dfrac{(p-1)}{2}y, \quad dy = \dfrac{2}{p-1}du$, and sech even,

$$\begin{aligned} b_m &= \frac{4}{p-1}\left(\frac{p+1}{2}\right)^{\frac{m}{p-1}} \int_0^{\infty} \operatorname{sech}^{\frac{2m}{p-1}}(u)du \\ &= \frac{4}{p-1}\left(\frac{p+1}{2}\right)^{\frac{m}{p-1}} \int_0^{\infty} \cosh^{\frac{-2m}{p-1}}(u)du. \end{aligned}$$

Let us express $\quad b_m \quad$ in terms of the Beta function using the steps described in Appendix B from [1].

$$\mathrm{B}(\mu,\nu)=\int_0^1 t^{\mu-1}(1-t)^{\nu-1}dt.$$

Using the fact that $\mathrm{B}(\mu,\nu)=\mathrm{B}(\nu,\mu)$ and the change of variable

$$y=\frac{1-t}{t}\Rightarrow t=\frac{1}{y+1}\Rightarrow dt=-\frac{1}{(y+1)^2}dy,$$

we obtain

$$\mathrm{B}(\mu,\nu)=\int_0^\infty\left(\frac{1}{y+1}\right)^{\nu+1}\left(\frac{y}{y+1}\right)^{\mu-1}dy.$$

For $y=t^2,\quad dy=2tdt,$

$$\mathrm{B}(\mu,\nu)=\int_0^\infty\left(\frac{1}{t^2+1}\right)^{\nu+1}\left(\frac{t^2}{t^2+1}\right)^{\mu-1}2tdt.$$

For $t=\sinh(y)\quad dt=\cosh(y)dy,$ we obtain

$$\mathrm{B}(\mu,\nu)=\int_0^\infty\left(\frac{1}{\sinh^2(y)+1}\right)^{\nu+1}\left(\frac{\sinh^2(y)}{\sinh^2(y)+1}\right)^{\mu-1}2\sinh(y)\cosh(y)dy.$$

$$\mathrm{B}(\mu,\nu)=2\int_0^\infty\cosh^{-2(\mu+\nu)+1}(y)\sinh^{2\mu-1}(y)dy.$$

For $\mu=\dfrac{1}{2},\quad$ and $\quad\nu=\dfrac{m}{p-1},\quad$ we have

$$b_m=\frac{2}{p-1}\left(\frac{p+1}{2}\right)^{\frac{m}{p-1}}\mathrm{B}\left(\mu,\nu\right)=\frac{2}{p-1}\left(\frac{p+1}{2}\right)^{\frac{m}{p-1}}\mathrm{B}\left(\frac{1}{2},\frac{m}{p-1}\right),$$

with the Beta function expressed in terms of the Γ function from definition 8.384 in [4] and defined as

$$\mathrm{B}\left(\mu,\nu\right)=\frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu+\nu)}.$$

Unlike its fellow, the Γ function is available in the C language, and this expression is designed to calculate precise values for the Beta function.

D) Let us prove that $\mathcal{L}_0$ is self-adjoint. We need to show $\Big\langle \mathcal{L}_0(u), v \Big\rangle = \Big\langle u, \mathcal{L}_0(v) \Big\rangle$, for all integrable functions u and v. Knowing that both u and $\partial_y u$ have exponential decay at infinity, we have

$$\begin{aligned}
\Big\langle \mathcal{L}_0(u), v \Big\rangle &= \int_{-\infty}^{\infty} \left(\partial_y^2 u - u + pu^{p-1}u\right) v dy = \int_{-\infty}^{\infty} v \cdot \partial_y^2 u dy + \int_{-\infty}^{\infty} \left(pu^{p-1}u - u\right) v dy \\
&= \Big[\partial_y u \cdot v\Big]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \partial_y u \cdot \partial_y v dy + \int_{-\infty}^{\infty} \left(pu^{p-1}u - u\right) v dy \\
&= -\Big[u \cdot \partial_y v\Big]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} u \cdot \partial_y^2 v dy + \int_{-\infty}^{\infty} \left(pu^{p-1}u - u\right) v dy \\
&= \int_{-\infty}^{\infty} \left(\partial_y^2 v - v + pu^{p-1}v\right) u dy = \Big\langle u, \mathcal{L}_0(v) \Big\rangle.
\end{aligned}$$

E) Expression of the Green's functions.
If we denote by G^- and G^+ the values of the Green's function in respectively $]-1, x_i[$ and $]x_i, 1[$. We can rewrite equations (3.21a) and (3.21b) as

$$DG_{xx}^+ - G^+ = -\delta(x - x_i), \quad G^+(1; x_i) = 0, \quad -1 < x < x_i, \tag{3.37a}$$

$$DG_{xx}^- - G^- = -\delta(x - x_i), \quad G^-(-1; x_i) = 0, \quad 0 < x < x_i, \tag{3.37b}$$

with $G^-(x; x_i) = G^+(x; x_i)$.
Homogeneous solutions:
The homogeneous equations of (3.37a) and (3.37b) are respectively

$$DG_{xx}^+ - G^+ = 0, \tag{3.38a}$$

$$DG_{xx}^- - G^- = 0. \tag{3.38b}$$

Characteristic equations:
Both (3.38a) and (3.38b) have the same characteristic equation
$r^2 - w_0^2 = 0, \quad$ with $\quad w_0^2 = \dfrac{1}{D}$.
$r^2 - w_0^2 = 0 \quad \Rightarrow \quad r = \pm w_0$, then, the solutions of the homogeneous equations are in $\text{span}\{e^{w_0 x}, e^{-w_0 x}\}$. In particular, we have

$$G^+ = A^+ \left(\frac{e^{w_0 x} + e^{-w_0 x}}{2}\right) + B^+ \left(\frac{e^{w_0 x} - e^{-w_0 x}}{2}\right) = A^+ \sinh(w_0 x) + B^+ \cosh(w_0 x), \tag{3.39a}$$

$$G^- = A^- \left(\frac{e^{w_0 x} + e^{-w_0 x}}{2}\right) + B^- \left(\frac{e^{w_0 x} - e^{-w_0 x}}{2}\right) = A^- \sinh(w_0 x) + B^- \cosh(w_0 x). \tag{3.39b}$$

with A^-, A^+, B^-, B^+ constants to be determined.
From (3.39a) and (3.39b), we have

$$G^+(1; x_i) = 0 \Rightarrow B^+ = -\tanh(w_0)A^+, \tag{3.40}$$

and

$$G^-(-1; x_i) = 0 \Rightarrow B^- = \tanh(w_0)A^-. \tag{3.41}$$

Substituting (3.40) and (3.41) in (3.39a) and (3.39b) leads to

$$G^+ = A^+ \operatorname{sech}(w_0)\cosh(w_0 x - w_0). \tag{3.42}$$

$$G^- = A^- \operatorname{sech}(w_0)\cosh(w_0 x + w_0). \tag{3.43}$$

Particular solution:

$$DG_{xx} - G = -\delta(x - x_i) \Rightarrow D\int_{x_i-\xi}^{x_i+\xi} G_{xx}dx - \int_{x_i-\xi}^{x_i+\xi} Gdx = -\int_{x_i-\xi}^{x_i+\xi} \delta(x - x_i)dx$$
$$\Rightarrow D\Big[G_x\Big]_{x_i-\xi}^{x_i+\xi} = -1.$$

Then,

$$G_x^+(x; x_i) - G_x^-(x; x_i) = -\frac{1}{D} \quad \Rightarrow \quad G_x^+(x; x_i) - G_x^-(x; x_i) = -w_0^2. \tag{3.44}$$

Replacing (3.42) and (3.43) in (3.44) leads to

$$A^+ \operatorname{sech}(w_0)\sinh(w_0 x_i - w_0) - A^- \operatorname{sech}(w_0)\sinh(w_0 x_i + w_0) = -w_0. \tag{3.45}$$

Using (3.44), (3.45) and the fact that $G^-(x; x_i) = G^+(x; x_i)$ leads to

$$A^- = A^+ \frac{\cosh(w_0 x_i - w_0)}{\cosh(w_0 x_i + w_0)}. \tag{3.46}$$

Substituting (3.46) in (3.47) gives

$$A^+ = \frac{w_0 \cosh(w_0 x_i + w_0)}{\operatorname{sech}(w_0)\sinh(2w_0)}, \tag{3.47}$$

and

$$A^- = \frac{w_0 \cosh(w_0 x_i - w_0)}{\operatorname{sech}(w_0)\sinh(2w_0)}. \tag{3.48}$$

Finally, (3.48) and (3.47) in (3.42) and (3.43) leads to

$$G^- = \frac{w_0 \cosh(w_0 x_i - w_0)}{\sinh(2w_0)}\cosh(w_0 x + w_0), \tag{3.49}$$

and

$$G^+ = \frac{w_0 \cosh(w_0 x_i + w_0)}{\sinh(2w_0)}\cosh(w_0 x - w_0). \tag{3.50}$$

F) Expression of the homoclinic solution u:

$$u'' - u + u^p = 0 \Rightarrow u''u' - uu' + u'u^p = 0 \Rightarrow \frac{1}{2}u'^2 - \frac{1}{2}u^2 - \frac{u^{p+1}}{p+1} = c_1.$$

Since $\lim_{|y|\to\infty} u = \lim_{|y|\to\infty} u' = 0, \qquad c_1 = 0$. This gives us

$$\frac{1}{2}u'^2 - \frac{1}{2}u^2 - \frac{u^{p+1}}{p+1} = 0. \tag{3.51}$$

Subsequently,

$$u'^2 = u^2 - \frac{2u^{p+1}}{p+1} \quad \Rightarrow \quad u' = \pm\sqrt{u^2 - \frac{2u^{p+1}}{p+1}}.$$

$$u' = \sqrt{u^2 - \frac{2u^{p+1}}{p+1}} \Rightarrow \frac{u'}{\sqrt{u^2 - \frac{2u^{p+1}}{p+1}}} = 1 \Rightarrow \int \frac{u'}{\sqrt{u^2 - \frac{2u^{p+1}}{p+1}}}dy = y + c_2.$$

Let $A = \int \frac{u'}{\sqrt{u^2 - \frac{2u^{p+1}}{p+1}}}dy$, and $\quad B = y + c_2$.

Since

$$u'dy = du,$$

we have

$$A = \int \frac{du}{\sqrt{u^2 - \frac{2u^{p+1}}{p+1}}} = \int \frac{du}{\sqrt{\frac{2}{p+1}}u^{\frac{p+1}{2}}\sqrt{\frac{p+1}{2}u^{1-p} - 1}}. \tag{3.52}$$

Substituting $\frac{p+1}{2}u^{1-p}$ with $\cosh^2(t)$ leads to

$$u = \left(\frac{2}{p+1}\right)^{\frac{1}{1-p}} \cosh^{\frac{2}{1-p}}(t), \qquad t = \operatorname{arccosh}\left(u^{\frac{1-p}{2}}\left(\frac{p+1}{2}\right)^{\frac{1}{2}}\right),$$

and

$$du = \frac{2}{1-p}\left(\frac{2}{p+1}\right)^{\frac{1}{1-p}} \sinh(t)\cosh^{\frac{p+1}{1-p}}(t)dt.$$

Substituting the previous results in (3.53) leads to

$$A = \int \frac{2}{1-p}dt = \frac{2}{1-p}t + c_2.$$

Equating A and B gives

$$t = \frac{p-1}{2}y + c_4. \tag{3.53}$$

For $y = 0$, $\quad t = \operatorname{arccosh}\left(u^{\frac{1-p}{2}}(0)\left(\frac{p+1}{2}\right)^{\frac{1}{2}}\right)$. From (3.51), we have

$$\frac{1}{2}u'^2 - \frac{1}{2}u^2 - \frac{u^{p+1}}{p+1} = 0 \Rightarrow u^2(0) = \frac{2u^{p+1}(0)}{p+1} \Rightarrow u^{1-p}(0) = \frac{2}{p+1}$$
$$\Rightarrow u^{\frac{1-p}{2}}(0) = \left(\frac{p+1}{2}\right)^{-\frac{1}{2}}.$$

Substituting the result in the expression of t results in

$$t = \operatorname{arccosh}(1) = 0 \quad \Rightarrow \quad c_4 = 0.$$

Subsequently,

$$\operatorname{arccosh}\left(u^{\frac{1-p}{2}}\left(\frac{p+1}{2}\right)^{\frac{1}{2}}\right) = \frac{p-1}{2}y,$$
$$u^{\frac{1-p}{2}}\left(\frac{p+1}{2}\right)^{\frac{1}{2}} = \cosh\left(\frac{p-1}{2}y\right),$$
$$u^{\frac{p-1}{2}} = \left(\frac{p+1}{2}\right)^{\frac{1}{2}} \operatorname{sech}\left(\frac{p-1}{2}y\right),$$

and then

$$u(y) = \left\{\left(\frac{p+1}{2}\right)\operatorname{sech}^2\left(\frac{p-1}{2}y\right)\right\}^{\frac{1}{p-1}}.$$

Chapter 4

Numerical Approximation of $\mathcal{D}_t^\gamma u$ with a Controlled Precision

4.1 Introduction, Method and Verification

4.1.1 Introduction and Background

As previously stated, the primary objective of this study is to numerically solve the one-dimensional Gierer-Meinhardt model with subdiffusion. By applying matched asymptotic expansion to the differential system (3.4), we have obtained an differential algebraic system (3.23). Our goal in addressing this system is to compute the quantities $\dfrac{dx_i}{d\sigma}$ and $H_i(\sigma)$, which represent the rates of change of spike positions and their respective heights. Monitoring both spike positions and heights enables us to identify regions where the activator and inhibitor significantly interact, as well as the differences in the magnitude of their concentrations. Our ability to determine these quantities within the system is primarily constrained by the computation of the fractional operator $\mathcal{D}_t^\gamma u$, defined as

$$\mathcal{D}_t^\gamma u(t) = \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right)\frac{1}{\Gamma(-\gamma)}\int_0^\infty \left\{u(t) - u\left(t + \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right)y\right)\right\}\left(\frac{1}{y}\right)^{\gamma+1} dy,$$

a task discussed in this section. The fractional operator $\mathcal{D}_t^\gamma u$ from (3.34) is an inherent part of this system. It is essential to compute it with consistent precision to prevent any form of contamination, since this term is only one of many in the numerical computation of (3.23), but the only one, whose accuracy is not immediately determined by a known numerical method. Hereunder, we chose t instead of y as in [6] as the dependent variable of $\mathcal{D}_t^\gamma u$ to symbolize its time dependency, as it is conceptually the case.

The fractional operator $\mathcal{D}_t^\gamma u$ depends on two parameters: p and γ, with p being a parameter related to the function u (main kinetic exponent for the activator equation). As shown in the next section, numerically computing $\mathcal{D}_t^\gamma u$ implies the integration of a spike-type fractional power function whose shape varies significantly, as shown in Figure 4.1 of section 4.1.5. Since that function is bell-shaped with a very steep slope, computing its integral requires a significant number of subdivisions. Moreover, since the spikes are defined in an infinite domain, the number of subdivisions required increases even further. Even though computing $\mathcal{D}_t^\gamma u$ requires a high number of subdivisions in all cases, their order of magnitude varies significantly depending on the shape of the spikes. For example, a normal spike with a bell width of order $\mathcal{O}(\epsilon)$ requires a number of subdivisions of order $\mathcal{O}(1/\epsilon)$. Moreover, the spike tail decays exponentially, which makes it easy to be captured in a relatively small interval. For instance, a spike of width 0.1 centered at the origin on a domain of $(-1, 1)$ will need $1/0.1 = 10$ subdivisions within $(-0.05, 0.05)$ to be properly captured.

An important consideration arises: any standard method of numerical integration provides an error bound that depends on the number of subdivisions. It is logical to question why we do not use such a formula to determine the number of subdivisions n based on the desired error. Let us explore this using Simpson's method as an example, which we will utilize further. According to [3, page 203], considering $f^{(4)}$ as the continuous fourth derivative of a function f, and M as any upper bound for the values of $|f^{(4)}|$ on $[a, b]$, the error $|E_f|$ in the Simpson's rule approximation of the integral of f from a to b satisfies the inequality:

$$|E_f| \leq \frac{(b-a)^5}{180}\frac{M}{n^4}.$$

However, this approach faces two primary challenges. Firstly, it involves M, supposedly the maximum for the fourth derivative of f. Yet, determining a maximum for a complicated function like $u^{(4)}$ is unfeasible. Secondly, an issue also arises with the term $b - a$. Operating within a theoretically infinite domain where a and b can tend to infinity, the term $b-a$ becomes an indeterminate form.

In summary, to efficiently compute $\mathcal{D}_t^\gamma u$, it is essential to find a way to determine the number of subdivisions required for controlled precision, depending on the shape of those spikes and the domain in which they are defined. Answering this question will be the subject of our study.

4.1.2 Procedure

1. We split $\mathcal{D}_t^\gamma u$ using two integrations by parts to simplify it and replace the original improper integral by proper computable terms.

2. The result of these integrations is a sum of constants and a yet-to-be-evaluated integral. We evaluate the integral using the composite Simpson method. We selected the C programming language due to its speed and efficiency, providing a significant advantage when dealing with memory-intensive and power-demanding data.

3. We gradually increment the number of subdivisions used by our program to compute these integrals until a precision of 10^{-10} is reached. These computations are performed for a predefined set of values of the parameters p and γ.

4. We attempted to plot the correspondence between the number of subdivisions n and the value of the integral obtained, but the resulting functions were neither smooth nor continuous. We then shifted our focus toward the residual function.

5. The shapes of the residual functions are similar to that of the hyperbolic arctangent function, which is then used as the fitting function.

6. Finally, we use the inverse functions of the fitting curves to approximate the number of subdivisions n given a residual value.

In summary, by implementing the above procedure, we expect to build a program capable of computing $\mathcal{D}_t^\gamma u$ for all values of p and γ with a precision of 10^{-10}.

4.1.3 Plan

1. Section 4.1.4 covers Step 1 in the procedure for regularizing $\mathcal{D}_t^\gamma u$.

2. Steps 2 and 3, starting from section 4.1.4 up to section 4.1.5, involve determining the number of subdivisions n needed to compute I (4.5). This calculation is for (t, p, γ) values within the ranges: $\{0.1, 1, 5\} \times \{1.5, 2, 2.5, \dots, 4.5\} \times \{0.1, 0.2, 0.3, \dots, 0.9\}$.

3. Steps 4, 5, and 6, spanning from section 4.1.5 to 4.1.6, describe the fitting process and can be visualized as follows:

   We fit the correspondence
   $$n_{(t,p,\gamma)} \to R_{(t,p,\gamma)}(n),$$
   using a variant of the hyperbolic-arctangent function, denoted as f. Consequently,
   $$n_{(t,p,\gamma)} \to f_{(t,p,\gamma)}(n) \sim R_{(t,p,\gamma)}.$$

   To find the number of subdivisions based on a specific residual (the inverse path), we determine the inverse f^{-1} of f so that
   $$f^{-1}_{(t,p,\gamma)}(R) \to n_{(t,p,\gamma)},$$
   where $n_{(t,p,\gamma)}$ and $R_{(t,p,\gamma)}$ represent the number of subdivisions and the corresponding residual values for specific t, p, and γ values.

4. The process is now generalized for $(t, p, \gamma) \in [0, 5] \times [1.5, 4.5] \times [0.1, 0.9]$ from section 4.1.7 to 4.1.8 using a series of linear and bi-linear interpolations.

5. Section 4.1.9 involves the verification process where the accuracy of our results is assessed.

4.1.4 Regularization of $\mathcal{D}_t^\gamma u$

This section serves as the first step of the plan outlined in section 4.1.3. It aims at removing the singularity inherent in the operator's $\mathcal{D}_t^\gamma u$ expression. From equation (3.34), we have

$$\mathcal{D}_t^\gamma u(t) = \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right)\frac{1}{\Gamma(-\gamma)}\int_0^\infty \left\{u(t) - u\left(t + \operatorname{sign}\left(\frac{dx_i}{d\sigma}\right)y\right)\right\}\left(\frac{1}{y}\right)^{\gamma+1} dy, \tag{4.1}$$

with

$$\mathcal{D}_{(-t)}^\gamma u(-t)\Big|_{\frac{dx_i}{d\sigma}>0} = -\mathcal{D}_t^\gamma u(t)\Big|_{\frac{dx_i}{d\sigma}<0}.$$

From (4.1), the expression of $\mathcal{D}_t^\gamma u$ is not directly computable because of the singularity present in the expression. Hence, we perform a double integration by parts and employ a Taylor expansion of u around a certain point to get rid of the singularity. For $\dfrac{dx_i}{d\sigma} < 0$ and $t > 0$, we have

$$\mathcal{D}_t^\gamma u(t) = -\frac{1}{\Gamma(-\gamma)}\int_0^{t_\infty}\frac{u(t) - u(t-y)}{y^{\gamma+1}}dy.$$

The first integration by parts

$$a(y) = u(t) - u(t-y), \quad \frac{db}{dy} = \frac{1}{y^{\gamma+1}},$$

leads to

$$\mathcal{D}_t^\gamma u(t) = -\frac{1}{\Gamma(-\gamma)}\left\{-\frac{u(t)-u(t-t_\infty)}{\gamma t_\infty^\gamma} + \lim_{y\to 0}\frac{1}{\gamma}\frac{u(t)-u(t-y)}{y^\gamma} + \int_0^{t_\infty}\frac{u'(t-y)}{\gamma y^\gamma}dy\right\},$$

with $\lim\limits_{y\to 0}\dfrac{u(t)-u(t-y)}{y^\gamma} = 0$. The proof for this is straightforward since

$$\frac{u(t)-u(t-y)}{y^\gamma} \sim \frac{u(t) - \left(u(t) + u'(t)(-y) + \dfrac{u''(t)y^2}{2!} + \cdots + \cdots\right)}{y^\gamma} = u'(t)y^{1-\gamma} - \frac{u''(t)y^{2-\gamma}}{2} + \cdots,$$

with $0 < \gamma < 1$. We obtain

$$\mathcal{D}_t^\gamma u(t) = -\frac{1}{\Gamma(-\gamma)}\left\{-\frac{u(t)-u(t-t_\infty)}{\gamma t_\infty^\gamma} + \int_0^{t_\infty}\frac{u'(t-y)}{\gamma y^\gamma}dy\right\}.$$

By applying a second integration by parts on the last terms in the brackets,

$$a(y) = u'(t-y), \quad \frac{db}{dy} = \frac{1}{y^\gamma},$$

we obtain

$$\int_0^{t_\infty} \frac{u'(t-y)}{\gamma y^\gamma} dy = -\frac{t_\infty^{1-\gamma}}{\gamma(\gamma-1)} u'(t-t_\infty) - \frac{1}{\gamma(\gamma-1)} \int_0^{t_\infty} u''(t-y) y^{1-\gamma} dy.$$

This finally leads to

$$\mathcal{D}_t^\gamma u(t) = -\frac{1}{\Gamma(-\gamma)} \left\{ -\frac{t_\infty^{-\gamma}}{\gamma} \left(u(t) - u(t-t_\infty)\right) - \frac{t_\infty^{1-\gamma}}{\gamma(\gamma-1)} u'(t-t_\infty) - \frac{1}{\gamma(\gamma-1)} \int_0^{t_\infty} u''(t-y) y^{1-\gamma} dy \right\}. \tag{4.2}$$

We have

$$-\gamma\Gamma(-\gamma) = \Gamma(1-\gamma) \text{ and } \gamma(\gamma-1)\Gamma(-\gamma) = \Gamma(2-\gamma).$$

Additionally, upon substituting $t-y$ with x, and then x with y, this leads to

$$\int_0^{t_\infty} u''(t-y) y^{1-\gamma} dy = -\int_t^{t-t_\infty} u''(y)(t-y)^{1-\gamma} dy.$$

We finally obtain

$$\mathcal{D}_t^\gamma u(t) = \frac{t_\infty^{-\gamma}}{\Gamma(1-\gamma)} \Big(u(t) - u(t-t_\infty)\Big) + \frac{t_\infty^{1-\gamma}}{\Gamma(2-\gamma)} u'(t-t_\infty) - \frac{1}{\Gamma(2-\gamma)} \int_t^{t-t_\infty} u''(y)(t-y)^{1-\gamma}\, dy. \tag{4.3}$$

Similarly, for $\dfrac{dx_i}{d\sigma} > 0$, and

$$\mathcal{D}_{(-t)}^\gamma u(-t)\Big|_{\frac{dx_i}{d\sigma}>0} = -\mathcal{D}_t^\gamma u(t)\Big|_{\frac{dx_i}{d\sigma}<0},$$

$$\begin{aligned} \mathcal{D}_{(-t)}^\gamma u(-t) = &-\frac{t_\infty^{-\gamma}}{\Gamma(1-\gamma)} \Big(u(t) - u(t-t_\infty)\Big) - \frac{t_\infty^{1-\gamma}}{\Gamma(2-\gamma)} u'(t-t_\infty) \\ &+ \frac{1}{\Gamma(2-\gamma)} \int_t^{t-t_\infty} u''(y)(t-y)^{1-\gamma}\, dy, \end{aligned}$$

with $0 < \gamma < 1$, and u defined as

$$u(t) = \left(\frac{p+1}{2} \operatorname{sech}^2 \frac{(p-1)t}{2}\right)^{\frac{1}{p-1}},$$

and verifying the following differential equation

$$u'' - u + u^p = 0, \quad -\infty < t < \infty. \tag{4.4a}$$

$$u'(0) = 0, \quad u(0) > 0, \quad \text{and} \quad \lim_{|t|\to\infty} u = 0. \tag{4.4b}$$

Let us have

$$I_1 = \frac{t_\infty^{-\gamma}}{\Gamma(1-\gamma)}\Big(u(t-t_\infty)-u(t)\Big), I_2 = \frac{t_\infty^{1-\gamma}}{\Gamma(2-\gamma)}u'(t-t_\infty),\ I_3 = \frac{t_\infty^{1-\gamma}}{\Gamma(2-\gamma)}\int_t^{t-t_\infty} u''(y)(t-y)^{1-\gamma}\,dy.$$

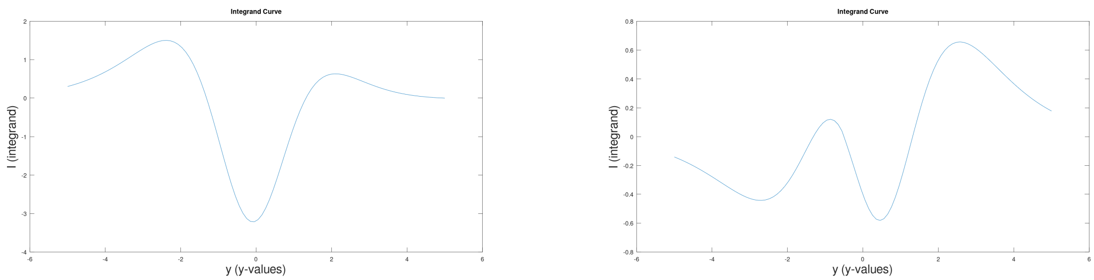
In both cases, $\mathcal{D}_t^\gamma u$ is expressed as the sum of three terms, the first two being constants, and the third being an integral. The first two terms are exact values, hence our approximation will focus solely on the integral. Furthermore, it is important to note that the integrand as well as the integration bounds remain the same for both $\dfrac{dx_i}{d\sigma} < 0$ and $\dfrac{dx_i}{d\sigma} > 0$. Therefore, the number of subdivisions required to compute the integral with the desired precision is the same in both cases. Hence, we will concentrate solely on determining

$$I = \int_t^{t-t_\infty} u''(y)(t-y)^{1-\gamma}\,dy, \tag{4.5}$$

for $\dfrac{dx_i}{d\sigma} < 0$.

4.1.5 Numerical Approximation of I with a Controlled Precision

In this section, along with subsequent sections up to 4.1.6, and in alignment with Step 2 of our plan, we determine the necessary number of subdivisions for the numerical computation of the integral I. The integrand of I depends on three parameters: p, γ, and t_∞. Based on extensive numerical trials and as demonstrated in the results section, the value of $t_\infty = 5$ has proved to be sufficient to approach I with the desired precision. In the subsequent subsections of this document, when referring to discrete values of p and γ, we respectively mean $p \in \{1.5, \ldots, 4.5\}$ and $\gamma \in \{0.1, \ldots, 0.9\}$. Conversely, when discussing continuous values of p and γ, we are referring to $p \in [1.5, 4.5]$ and $\gamma \in [0.1, 0.9]$. As mentioned earlier, the shape and gradient exhibit significant variation based on these parameters, influencing the number of subdivisions required for computation. To streamline the process and avoid redundant calculations of I, we seek a method to predict the necessary number of subdivisions and assess precision as we compute the integral. Below are the curves of the integrand for some values of the parameters.



(a) $u''(y)(t-y)^{1-\gamma}$ for $t=5$ (b) $u''(y)(t-y)^{1-\gamma}$ for $t=0.5$

Figure 4.1: Plots of $u''(t)(t-y)^{1-\gamma}$ for $p=2$, $\gamma=0.1$ for $t=5$(right) and $t=0.5$(left). The horizontal axis represents range of y-values and the vertical axis the corresponding integrand values.

Computing I using the composite Simpson's method

In addition to being a well-established and widely used numerical integration method, we chose the composite Simpson's method for its adaptability. The composite Simpson's method can be applied to both evenly and unevenly spaced intervals, making it versatile for various types of functions and integration domains. This adaptability allows for efficient integration over complex domains or functions with irregular behavior. The following algorithm from [3, page 204] is used to compute the integral I:

$$\int_a^b f(x)dx \approx \frac{h}{3}\sum_{i=0}^{n/2-1}\Big[f(x_{2i})+4f(x_{2i+1})+f(x_{2i+2})\Big], \quad \text{with} \quad h=\frac{b-a}{n}.$$

Implementation of the Simpson's method in C: The method computes the integral of the function named `integrand` using the composite Simpson's method. Here, `integrand` represents the actual integrand of I. Parameter list:

- `lower`: lower bound of the integral.
- `upper`: upper bound of the integral.
- `subInterval`: number of sub-intervals.
- `g`: gamma parameter.
- `A = pow((p+1.0)/2.0, 1.0/(p-1.0))`.
- `B = 2.0/(p-1.0)`.
- `C = (p-1.0)/2.0`.

Process:

- Calculate the step size.
- Sum the image by `integrand` of the lower and upper bounds of the integral first.
- Add the images by `integrand` of the values between the lower and upper bounds depending on whether the discretization index is odd or even.
- Multiply the result by one-third of the `stepSize`.

```



double simpson(double lower, double upper, long int subInterval, double p, double g) {

  double stepSize = (upper - lower) /( subInterval);

  int i;
  double integration = integrand(lower, p, g, y) + integrand(upper, p, g, y);
  for (i = 1; i <= subInterval - 1; i++) {
    double k = lower + i * stepSize;
    if (i % 2 == 0) {
      integration = integration + 2 * integrand(k, p, g, y);
    } else {
      integration = integration + 4 * integrand(k, p, g, y);
    }
  }
  integration = integration * stepSize / 3;
  return integration;

}
  // implementation of the integrand

double integrand(double y, double p, double g, double t) {

  return (u(y, p) - pow(u(y, p), p)) * pow(t - y, 1 - g);

}

// implementation of u

double u (double t,double p)
{
    double A = pow( (p+1.0)/2.0, 1.0/(p-1.0));
    double B =  2.0/(p-1.0);
    double C = (p-1.0)/2.0;
```

```

    return (A*pow(sech(C*t), B));
}
```

Listing 4.1: Implementation of the composite Simpson method with its dependencies in C

Note: The number of `subInterval` used by the Simpson method must be even. Lines 48 to 50 from Listing 4.10 always ensure it is the case.

Computing and printing the result of the Simpson method using the `WriteFile` method: To enhance readability, we have opted to display the return values of the integral I alongside the corresponding number of subdivisions needed for its calculation, as shown in Table 4.4. This formatting enables us to gather and analyze the data more efficiently.

For each combination of t, p, and γ, the `WriteFile` method creates a file and prints, side by side, the return values of the Simpson method with their corresponding number of subdivisions until the desired precision is reached. Considering that we are handling very large values of n, and only the last values of n are of interest, we double the increment value each time we run the first loop until we reach a precision of 5×10^{-10}. Once that precision is achieved, new values of the increments are used until 1×10^{-10} is reached. The value of the increments used in the second loop is returned by the `getIncrement` function and represents 5% of the number of subdivisions required to reach the 5×10^{-10} precision in the first loop. This `WriteFile` function is used to print the returned value of the Simpson method for discrete values of $p \in \{1.5, \ldots, 4.5\}$ and $\gamma \in \{0.1, \ldots, 0.9\}$.

Parameter list:

- `p`: discrete values of p.
- `g`: discrete values of γ.
- `t`: $\in \{0.1, 1, 5\}$.
- `n`: max number of subdivisions allowed.

Process:

- Extract the integer and decimal part of `p` and `g`.
- Write or create a file for a specific combination of `p` and `g` where the returned value of the Simpson method will be printed.
- Run the first loop and double the increment until $1 \times 10^{-10} <$ `error` $< 5 \times 10^{-10}$.
- Run the second loop with a custom increment until `error1` $< 10^{-10}$.
- `error` and `error1` are expresed as `Simpson(lower, upper, n) - Simpson(lower, upper, 2n)`.

Please note that "`Simpson(lower, upper, n)`" represents the result of the Simpson method with the given parameters `lower`, `upper`, and `n`.

```c
void writeFile(double p, double g, double t, long int n) {

  double A = pow((p + 1.0) / 2.0, 1.0 / (p - 1.0));
  double B = 2.0 / (p - 1.0);
  double C = (p - 1.0) / 2.0;
  double upper = t;
  double tmax = 5;
  double lower = t-tmax;

  int int_g = 10 * g;
  double p1 = (int) p;
  double p2 = 10 * (p - p1);
  long int i = 0;

  double g1 = (int) g;
  double g2 = 10 * (g - g1);
  long int increment = 1000;
  long int next;
  double precision1 = 5e-10;
  double precision2 = 1e-10;

  long int j;
  char str_i[25];
  FILE * diag;
  FILE * diag1;

  sprintf(str_i, "p%0.0fp%0.0f_g%0.0fp%0.0f.txt", p1, p2, g1, g2);

  diag = fopen(str_i, "a");
  if (!diag) {
    printf("Failed to open diagonal dominance file.\n");

  }

  for (i = 1000; i < n; i += i) {

    double value = simpson(lower, upper, i, g, A, B, C);

    double value5 = simpson(lower, upper, 2 * i, g, A, B, C);

    double error = fabs(value - value5);

```

```c
    if (error > precision1) {

      fprintf(diag, "%ld %0.15f\n", i, value5);
    } else if (error <= precision1 && error > precision2) {
      next = i;
      break;
    }

  }

 increment = getIncrement (t, p, g); // Find the increment depending on t, p and gamma

  for (j = next; j < n; j += increment) {

    double value1 = simpson(lower, upper, j, g, A, B, C);

    double value10 = simpson(lower, upper, 2 * j, g, A, B, C);

    double error1 = fabs(value1 - value10);

    if (error1 < precision2) {

      break;
    } else {

      fprintf(diag, "%ld %0.15f\n", j, value10);

    }

  }

  fclose(diag);
}
```

Listing 4.2: Implementation `WriteFile` method in C

Number of subdivisions returned by the `WriteFile` method for $t = 0.1$, 1 and 5: Once the desired precision is achieved, the final line printed by the `WriteFile` function contains the return value of the Simpson method with the correct precision, along with the corresponding number of subdivisions necessary to attain that precision. The tables below present the maximum number of subdivisions for each t, p, and γ.

p/g	1.5	2.0	2.5	3.0	3.5	4.0	4.5
0.1	35290	51740	61610	73870	80450	87030	93610
0.2	99900	135800	163900	199800	217750	235700	253650
0.3	216940	344940	433880	522820	567290	611760	689880
0.4	609778	865778	1101630	1377778	1495704	1731556	1849482
0.5	1693204	2362408	3386408	3721010	4390214	5059418	5394020
0.6	4718250	7300300	9970550	12464400	14066550	15668700	17270850
0.7	16113048	28265572	38166882	46087930	54550882	60491668	68412716
0.8	76333764	132864908	182371458	223956960	263749554	301374532	333058724
0.9	383072000	730144000	1018144000	1028288000	1028288000	1028288000	1028288000

Table 4.1: Number of subdivisions for $t = 0.1$

p/g	1.5	2.0	2.5	3.0	3.5	4.0	4.5
0.1	28000	26500	11000	22000	32500	39500	42500
0.2	71900	67550	23900	55700	83750	103500	111400
0.3	175500	166000	60500	130500	204000	251500	280000
0.4	444800	397600	134800	316800	515600	633600	700800
0.5	1141700	1078730	318970	826850	1393580	1716670	1905580
0.6	3547200	3172400	886800	2335800	4109400	5233800	5983400
0.7	11817400	10530500	2691450	7956700	14626500	18487200	21061000
0.8	52417200	46626150	12460850	34400600	63653600	83600550	95826100
0.9	260332000	232504000	44212000	162934000	325868000	451094000	506750000

Table 4.2: Number of subdivisions for $t = 1$

p/g	1.5	2.0	2.5	3.0	3.5	4.0	4.5
0.1	17100	11600	9100	8000	7300	6900	6600
0.2	42200	28000	21700	18800	17300	16100	15500
0.3	98200	63800	48800	41600	38200	35800	34000
0.4	234500	146500	110500	94000	84500	78500	75500
0.5	596400	364800	268600	227900	202000	187200	178700
0.6	1684000	992000	716000	596000	526000	486000	456000
0.7	5458000	3070000	2171000	1768000	1566000	1442000	1349000
0.8	21119000	11412000	7847000	6357000	5551000	5055000	4714000
0.9	101674000	51754000	34392000	27318000	23650000	21292000	19720000

Table 4.3: Number of subdivisions for $t = 5$

Fitting the residual R instead of the integral I

The fitting process begins from this paragraph and extends to the end of this section, aligning with Stage 3 of our plan. In accordance with the plan, an initial attempt was made to directly manipulate the integral values I; however, the resulting plots exhibited neither smoothness nor continuity. Consequently, the decision was made to utilize the residual R instead.

Upon execution of the `WriteFile` method, output files are generated, containing two columns: the first column denotes the number of subdivisions, while the second column displays the return values yielded by the Simpson method. Table 4.4 provides an illustration of a sample file produced by the `WriteFile` function for $t = 1$, $p = 4$, and $\gamma = 0.8$.

Given our objective to determine the number of subdivisions required to achieve a specific level of precision or error, it is logical to establish a relationship between N and the error or residual (i.e., the difference between the last value printed by the `WriteFile` function and the preceding values). Table 4.5 represents an updated version of Table 4.4, now featuring residual values as the second column.

The fitting process spans across three files: `test1.m`, `fit_curve.m`, and `fit_curvef.m`, which are described subsequently.

N	I
75879150	-0.590274039200124
76522600	-0.590274039199605
77166050	-0.590274039198941
77809500	-0.590274039197867
78452950	-0.590274039197240
79096400	-0.590274039196180
79739850	-0.590274039195590
80383300	-0.590274039194982
81026750	-0.590274039194301
81670200	-0.590274039193123
82313650	-0.590274039192075
82957100	-0.590274039191671
83600550	-0.590274039191116

Table 4.4: Integral values

N	R
75879150	$1.2251e-11$
76522600	$1.0456e-11$
77166050	$9.9369e-12$
77809500	$9.2729e-12$
78452950	$8.1990e-12$
79096400	$7.5719e-12$
79739850	$6.5120e-12$
80383300	$5.9219e-12$
81026750	$5.3140e-12$
81670200	$4.6330e-12$
82313650	$3.4550e-12$
82957100	$2.4070e-12$
83600550	$2.0030e-12$

Table 4.5: Residual values

Inside the `test1.m` file: During the fitting process of the residual function, we opted for the logarithm of the residual instead of the actual residual function. In fact, the residual function is a power function, which implies that its values are either extremely small or large over most of its domain. Attempting to gain insights from its plot has proven to be quite challenging. Also, the fit would be highly non-uniform. For example, how do we ensure that the small values are fit as well as the large values? How do we measure what is a good fit when the disparity in magnitude is so great? The log is the answer: it turns a very strongly varying power function into quasi-straight lines. Straight lines are simpler to handle in terms of quantifying their properties. If the original function is not a single power (which is our case), the log would not be a straight line, but the magnitude disparity issue is resolved nonetheless. The other aspect of it all is that we are indeed interested in the error magnitude, not its absolute value. We will always describe the residual as a magnitude. Thus, the log treatment also makes sense conceptually, beyond being a technical convenience. In the subsequent sections of the document, when we mention the residual function, we are actually referring to its logarithm. Process:

- Extract the integer and decimal parts of `p` and `g` and convert them into strings.

- Open the file printed by the `WriteFile` function for that specific combination of `p` and `g`.
- Load this file into the vector `U`.
- Compute the residual function.
- Fit the residual function.
- Plot the results.

In the context of the `test1.m` file, the goal is to establish a functional relationship between the number of subdivisions N and the error or residual R for a given combination of p and γ. By fitting the plot of the residual against the number of subdivisions with a continuous and easily invertible function, the program can determine the number of subdivisions required to achieve a specific precision.

```

for p=1.5:0.5:4.5
  for g = 0.1:0.1:0.9

  %extract the integer and decimal part of p

   p1=fix(p);
   p2=10*(p-p1);

%extract the integer and decimal part of g
   g1=fix(g);
   g2=10*(g-g1);

%convert them into strings
   sp1=num2str(p1);
   sp2=num2str(p2);
   sg1=num2str(g1);
   sg2=num2str(g2);

%open the file containing the return value of the WriteFile
% method depending on a sepcific combination of p and g


file=['C:/Users/nguim/OneDrive/Documents/research_papers
/Code/newdata/P_G/t5/p' sp1 'p' sp2 '_g' sg1 'p' sg2 '.txt'];

% load the file as a 2 dimoentional vector
   U=load(file);

   N=U(:,1); % the vector N contains the subdivisions
```

```
    G=U(:,2); % the vector G contains the actual return value the
        WriteFile method

  % R is the residual vector containing the difference between the last
      value of G and the other ones
  %
    R=log10(abs(G(1:end-1)-G(end)));
    N=N(1:end-1);

% c is a parameter vector that will minimizes the euclidian distance
    between
% the Residual functions and their fitted curves
    c0=[-1 -6]; % initial parameter of the fminunc function
    c=fminunc(@(c) fit_curve(c,R,N), c0);

    [f,imin,imax]=fit_curvef(c,N);
    N1=N;
    N1([imin imax])=[];
    plot(N,R,N1,f,'--');
    hold on

  endfor
endfor
```

Listing 4.3: Fitting the residual function.

Inside the `fit_curvef.m` file: The function `fit_curvef` is tasked with fitting the residual using the general form of the atanh function, $c_1 \operatorname{atanh}(n_1) + c_2$, by determining optimal values for the scaling factor c_1, the slope n_1, and the vertical shift c_2.

Parameters list:

- `c`: a two-dimensional vector.
- `n`: the number of subdivisions.

Process:

- Get the minimum value of the vector `n`.
- Get the maximum value of the vector `n`.
- Remove these extreme values from the vector `n`.
- Determine the fitting curve using the parameter `c`.

```
function [f,imin,imax]=fit_curvef(c,n)

[minn,imin]=min(n);
[maxn,imax]=max(n);
n([imin imax])=[];
n1=2*(n-minn)/(maxn-minn)-1;
f=c(1)*atanh(n1)+c(2);
```

Listing 4.4: Implementation of the `fit_curvef` method .

Inside the `fit_curve.m` file: The `fit_curve` function returns the Euclidean distance between the residuals and their fitting curves. Specifically, the parameters c_1 and c_2 are selected to minimize this Euclidean distance.
Parameters list:

- `c`: a two-dimensional vector returned by the `fminunc` function.
- `u`: the function being fitted; in our case, it represents the residual function.
- `n`: represents the number of subdivisions.

Process:

- Call the `fit_curvef` function and pass into it the vector `c`.
- `fit_curvef` returns the fitting curve `f`, as well as `Imax` and `Imin`, which respectively represent the maximum and minimum values of `n`.
- Remove `Imax` and `Imin` from `n`.
- Determine the Euclidean distance between the fitting curve `f` and `u`.

```
function R=fit_curve(c,u,n)

[f,imin,imax]=fit_curvef(c,n);
u([imin imax])=[];
R=sqrt(sum((f-u).^2));
```

Listing 4.5: Implementation of the `fit_curve` method.

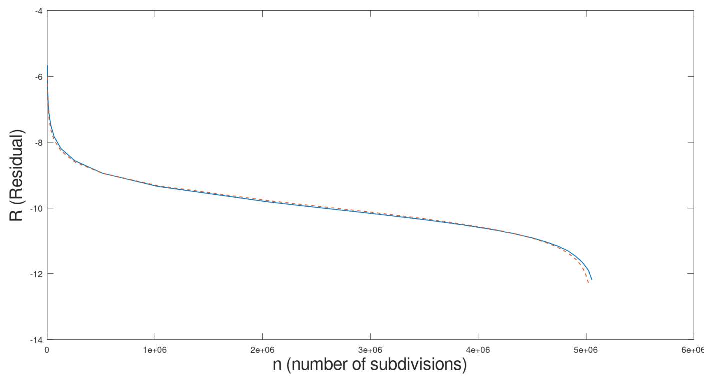


Figure 4.2: specific case for $t = 5$, $p = 4$, and $\gamma = 0.8$. The x-axis represents the number of subdivisions and the y-axis the logarithm of the corresponding residuals. The solid curve represents the numerical results while the dashed one represents the fitting curve.

Interpolation of the number of subdivisions N using the fitting curve

Once completing the fitting with the `atanh` function , its inverse can now be utilised to determine the corresponding R for every value of n. From the `fit_curvef.m` file, we have $n_1 = \dfrac{2 \times (n - \text{minn})}{(\text{maxn} - \text{minn})} - 1$ and $R \equiv f = c_1 \times \text{atanh}(n_1) + c_2$. The inverse process leads to $n_1 = \dfrac{\tanh(f - c_2)}{c_1}$ and $n = \dfrac{(n_1 + 1) \times (\text{maxn} - \text{minn})}{2} + \text{minn}$. This expression is used in the `n_approx` function to approximate the number of subdivisions n as subsequently explained.

Inside the `n_approx` function: The function `n_approx` iterates through the data files and substitutes the variables R, c_1, c_2, maxn, and minn in the expressions $n_1 = \dfrac{\tanh(f - c_2)}{c_1}$ and $n = \dfrac{(n_1 + 1) \times (\text{maxn} - \text{minn})}{2} + \text{minn}$ with their corresponding values given the parameters t, p, and γ. It calculates and returns the number of subdivisions `n` given `t`, `p`, `g`, and the residual `R`.

Parameters list:

- `t`: upper bound of the integral.
- `p`: between 1.5 and 4.5 with an increment of 0.5.
- `g`: between 0.1 and 0.9 with an increment of 0.1.
- `R`: the residual value.

Process:

- Load the `c.txt` containing the different values of the `c` vector for a given `t`.
- Load the `Nmax_Nmin.txt` file containing the maximum and minimum number of subdivisions for a given `t`.
- Compute `n` using the new formula.

```
double n_approx(double t, double p, double g) {

  double n1, n, pos_p, pos_g;
  FILE * fp1;
  FILE * fp2;
  FILE * fp3;
  char file_name1[25];
  char file_name2[33];
  char file_name3[25];
  float c1 = 0, c2 = 0, nMax = 0, nMin = 0, R;
  char * param;
  int i = 0, location = 0;

  pos_p = 1 + (p - 1.5) / 0.5;
  pos_g = g / 0.1;

  // find the location of c1 and c2 in the C.txt file as well as the location of Nmax and Nmin in the N.txt file knowing p and g

  location = (int)((pos_p - 1) * 9 + pos_g);

  // assign a value to param based on the value of t

  if (t == 0.1) {
    param = "0p1";
  } else if (t == 1) {
    param = "1";
  } else  {
    param = "5";
  }

  // create a path to the C.txt, N.txt, and R.txt files using the param variable

  sprintf(file_name1, "../../Data/C/t%s/C.txt", param);
  sprintf(file_name2, "../../Data/Nmax_Nmin/t%s/N.txt", param);
  sprintf(file_name3, "../../Data/R/t%s/R.txt", param);

  // open N.txt, C.txt, and R.txt

```

```
  fp1 = fopen(file_name1, "r");
  fp2 = fopen(file_name2, "r");
  fp3 = fopen(file_name3, "r");

  if (!fp2) {
    printf("fail_2");
  }

  if (!fp1) {
    printf("fail_1");
  }
  if (!fp3) {
    printf("fail_3");
  }

  for (i = 0; i < location; i++) {
    fscanf(fp1, "%f %f  ", &c1, &c2); // find c1 and c2 using the location variable
    fscanf(fp2, "%f %f  ", &nMin, &nMax); // find nMin and nMax using the location variable
    fscanf(fp3, "%f ", &R); // find R  using the location variable

  }


  fclose(fp1);
  fclose(fp2);

  n1 = tanh((R - c2) / c1);
  n = ((n1 + 1) * (nMax - nMin)) / 2 + nMin; // find n

  return n;

}
```

Listing 4.6: Implementation of the `n_approx` method.

Number of subdivisions obtained by executing `n_approx` for $t = 0.1$, 1, and 5: Tables 4.6, 4.7, and 4.8 display the approximate number of subdivisions returned by the `n_approx` function for $t = 0.1$, $t = 1$, and $t = 5$. Having a program capable of predicting the number of subdivisions n required to compute I for discrete values of $t \in \{0.1, 1, 5\}$, $p \in \{1.5, \ldots, 4.5\}$, and $\gamma \in \{0.1, \ldots, 0.9\}$, we intend to expand the program's scope to encompass continuous values of $t \in [0, 5]$, $p \in [1.5, 4.5]$, and $\gamma \in [0.1, 0.9]$. To achieve this, we will gradually transition from discrete to continuous values, starting with t in the subsequent section.

g/p	1.5	2.0	2.5	3.0	3.5	4.0	4.5
0.1	35065	51414	61242	73570	80108	86651	93201
0.2	99002	134710	162937	198630	216504	234382	252262
0.3	214565	342453	430919	519457	563799	608143	686814
0.4	602747	858551	1093366	1370345	1487766	1722571	1840192
0.5	1674913	2341552	3365120	3698389	4365537	5033725	5366720
0.6	1674913	7241978	9904136	12403810	13999256	15597980	17196034
0.7	4662043	28071526	37953058	45866233	54342976	60260601	68207443
0.8	15930379	132684487	182123946	223677191	263586831	301086078	332831576
0.9	76155108	727802772	1015373018	1025834015	1025841827	1025918580	1025859852

Table 4.6: Approximated number of subdivisions for $t = 0.1$

g/p	1.5	2	2.5	3.0	3.5	4.0	4.5
0.1	27873	26378	10927	21895	32362	39371	42358
0.2	71597	67150	23662	55344	83377	103044	110919
0.3	174554	165106	59775	129525	202917	250255	278688
0.4	442094	395096	132836	314216	512656	630341	697983
0.5	1134337	1071579	313754	820575	1385528	1708829	1897254
0.6	1134337	3153872	871089	2317025	4088223	5210846	5958598
0.7	3527550	10468585	2640180	7900759	14564452	18417018	20991875
0.8	11753526	46563914	12411139	34340174	63593768	83514848	95754535
0.9	52352342	231613175	43366292	162079821	324972385	449967670	505825475

Table 4.7: Approximated number of subdivisions for $t = 1$

g/p	1.5	2.0	2.5	3	3.5	4.0	4.5
0.1	17083	11585	9085	7986	7286	6886	6586
0.2	42163	27968	21670	18772	17273	16074	15474
0.3	98128	63737	48741	41544	38147	35748	33949
0.4	234320	146338	110344	93857	84362	78364	75366
0.5	595947	364389	268200	227526	201649	186865	178355
0.6	595947	990878	714928	595009	525021	485046	455084
0.7	1682968	3066607	2168010	1765265	1563165	1439166	1346239
0.8	5453895	11407642	7844868	6353968	5548342	5052182	4711303
0.9	21115912	51737121	34370523	27302158	23631082	21275601	19703359

Table 4.8: Approximated number of subdivisions for $t = 5$

4.1.6 Number of Subdivisions Required to Compute I for Continuous Values of t and Discrete Values of p and γ

This section up to section 4.1.8, corresponding to step 4 of the plan, signifies the transition from discrete values of parameters p, t, and γ to continuous values, achieved through a series of interpolations. We utilize linear interpolation to extend the scope of our program to handle continuous values of t. For optimization purposes, we implement four different variants of linear interpolation formulas and select the most conservative one, which returns the highest value of n. For $t \in [t_1, t_2]$, their general formulas are:

1. $n_t = n_{t_1} + \frac{(t-t_1)(n_{t_2}-n_{t_1})}{(t_2-t_1)}$,
2. $n_t = n_{t_1} + \frac{(\log(t)-\log(t_1))(n_{t_2}-n_{t_1})}{(\log(t_2)-\log(t_1))}$,
3. $\log(n_t) = \log(n_{t_1}) + \frac{(t-t_1)(\log(n_{t_2})-\log(n_{t_1}))}{(t_2-t_1)}$,
4. $\log(n_t) = \log(n_{t_1}) + \frac{(\log(t)-\log(t_1))(\log(n_{t_2})-\log(n_{t_1}))}{(\log(t_2)-\log(t_1))}$,

with log referring to the $\log_{10}$ function.

Implementation of these variants in C

Below are their respective implementation in C.

```c


int N_T(double t, double t1, double t2, int n1, int n2)
{
   int  n = (int)(n1 + (t - t1)*(n2 - n1)/(t2 - t1));
   return n;
}

int N_logT(double t, double t1, double t2, int n1, int n2)
{
   int n = (int)(n1 + (log10(t) - log10(t1))*(n2 - n1)/(log10(t2) -
      log10(t1)));
   return n;
}

int logN_T(double t, double t1, double t2, int n1, int n2)
{
   double logn = log10(n1) + (t - t1)*(log10(n2)-log10(n1))/(t2 - t1);
   return (int)(pow(10, logn));
}

int logN_logT(double t, double t1, double t2, int n1,  int n2)
{
   double logn = log10(n1) + (log10(t) - log10(t1))*(log10(n2)- log10(
      n1))/
   (log10(t2) - log10(t1));
   return (int)(pow(10, logn));
}
```

Listing 4.7: Implementation of the previous interpolation functions in C.

Determining the most conservative linear interpolation method using the `linearN_T` function

The purpose of `linearN_T` is straightforward: it compares the values of the number of subdivisions returned by each method and returns the highest one.

```
int linearN_T(double t, double t1, double t2, int n1, int n2)
{
  int   temp1 = N_T(t, t1, t2, n1, n2);
  int  temp2 = N_logT(t,t1, t2, n1, n2);
  int   temp3 = logN_T(t, t1, t2,  n1, n2);
  int   temp4 = logN_logT(t, t1, t2,  n1, n2);

  int n = temp1;

  if (n < temp2)
  {
    n = temp2;
  }

  if (n < temp3)
  {
    n = temp3;
  }

  if (n < temp4)
  {
    n = temp4;
  }

  return n;
}
```

Listing 4.8: Code used to compare the different interpolation methods.

4.1.7 Number of Subdivisions Required to Compute I with a Controlled Precision for Continuous Values of t, p and γ

In contrast to t, the transition from discrete to continuous values for the pair of parameters (p, γ) is accomplished using bi-linear interpolation. This is because (p, γ) constitute a pair of parameters, unlike t, which is a single parameter. For a given (p, γ) such that $p_1 \leq p \leq p_2$ and $\gamma_1 \leq \gamma \leq \gamma_2$, we aim to determine its corresponding number of subdivisions n. Below are the bi-linear interpolation formula and its implementation in our code.

Bi-linear interpolation formula

$n = \frac{\gamma-\gamma_2}{\gamma_1-\gamma_2}\left(\frac{n_{p_1,\gamma_1}(p-p_2)}{p_1-p_2} + \frac{n_{p_2,\gamma_1}(p-p_1)}{p_2-p_1}\right) + \frac{\gamma-\gamma_1}{\gamma_2-\gamma_1}\left(\frac{n_{p_1,\gamma_2}(p-p_2)}{p_1-p_2} + \frac{n_{p_2,\gamma_2}(p-p_1)}{p_2-p_1}\right).$

Implementation in C

```c

int bilinearN_p_g(double p, double g, double t) {

  int n;
  double p1, p2, g1, g2;
  double n_p1g1, n_p1g2, n_p2g1, n_p2g2;

  findPosition_p(p, &p1, &p2); // find p1
  findPosition_g(g, &g1, &g2); // find p2

  n_p1g1 = n_approx(t, p1, g1); // find n for p=p1 and g=g1
  n_p1g2 = n_approx(t, p1, g2); // find n for p=p1 and g=g2
  n_p2g1 = n_approx(t, p2, g1); // find n for p=p2 and g=g1
  n_p2g2 = n_approx(t, p2, g2); // find n for p=p2 and g=g2

  // find n

  n = (int)((g - g2) / (g1 - g2) * (n_p1g1 * (p - p2) / (p1 - p2) + n_p2g1* (p - p1) / (p2 - p1))
  + (g - g1) / (g2 - g1) * (n_p1g2 * (p - p2) / (p1 - p2) + n_p2g2 * (p - p1) / (p2 - p1)));

  return n;
}
```

Listing 4.9: Bi-linear interpolation of n in C.

4.1.8 Summary of the Interpolation Process

The previously encountered interpolation processes, either linear or bilinear, are part of a new function called `n_approx_general`, which can be regarded as an extension of `n_approx` to real values of t, p, and γ.

On one hand, `n_approx` allows us to predict the number of subdivisions required to approximate I for discrete values of t, p, and γ. On the other hand, `n_approx_general` performs the same task but over their continuous range.

The process to find the number of subdivisions required for an unknown triplet (t, p, γ) involves finding two triplets (t_1, p_1, γ_1) and (t_2, p_2, γ_2) such that $t_1 \leq t \leq t_2$, $p_1 \leq p \leq p_2$, and $\gamma_1 \leq \gamma \leq \gamma_2$. Moreover, it finds n_1 required for (t_1, p_1, γ_1) and n_2 required for (t_2, p_2, γ_2), and then computes n required for (t, p, γ) using interpolation.

This comprehensive approach allows us to efficiently estimate the number of subdivisions needed to achieve the desired precision for the integral over a wider range of input values.

Algorithm of the `n_approx_general` function

Algorithm 1: `n_approx_general` Algorithm

Result: Find n for continuous values of t, p and γ
;
if $t \in \{0.1, 1, 5\}$ **then**
  n = bilinear(t, p, γ) ;
end
else
  find $(t_1, t_2) \in \{0.1, 1, 5\} \times \{0.1, 1, 5\}$ such that $t_1 \leq t \leq t_2$;
  n1 = bilinear(t1, p, γ) ;
  n2 = bilinear(t2, p, γ) ;
  n = linear(t, t1, n1, t2, n2) ;
end

Implementation in C of the `n_approx_general` function

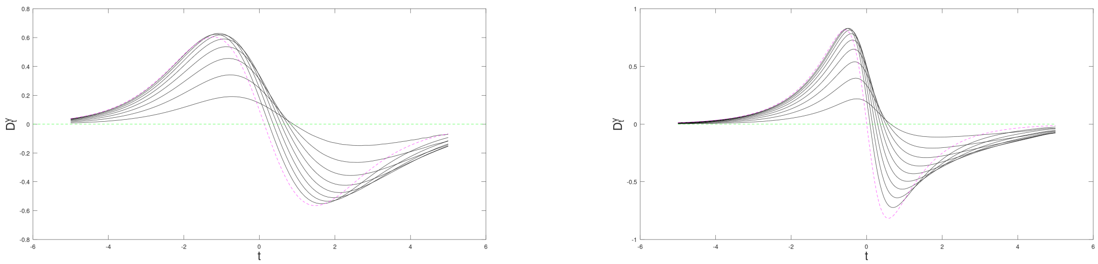
```c
int n_approx_general(double t, double p, double g) {

  double t1, t2;

  double p1 = (int) p; // extract the integer part of p
  double p2 = 10 * (p - p1); // extract the decimal part of p
  long int i = 0;
  double g1 = (int) g; // extract the integer part of g
  double g2 = 10 * (g - g1); // extract the decimal part of p

  int n, n1, n2;

  // if t is not in the set {0, 0.1, 1, 5}, find t1 and t2 such that t1
      <= t<= t2

  if (t != 0.1 && t != 5 && t != 1 && t != 0) {
    t1 = 0.1;
    t2 = 10;

    if (t < 1) {
      t1 = 0.1;
      t2 = 1;
    } else if (1 < t < 5) {
```

```
      t1 = 1;
      t2 = 5;
    } else {
      t1 = 0.1;
      t2 = 5;
    }

    n1 = bilinearN_p_g(p, g, t1); // find n for p, g and t1 using bilinear interpolation
    n2 = bilinearN_p_g(p, g, t2); // find n for p, g and t2 using bilinear interpolation

    n = linearN_T(t, t1, t2, n1, n2); // find n knowing n1 and n2 using linear interpolation

  } else if (t == 0) // find n for t=0
  {
    t = 0.1;
    n = bilinearN_p_g(p, g, t) + 1;

  } else {

    // if t is  in the set {0.1, 1, 5} use bilinear interpolation to compute it directly
    n = bilinearN_p_g(p, g, t);

  }
  // verify that n is even, because the composite Simpson method only works with even values of n.

  if (n % 2 != 0) {
    n += 1;
  }

  return n;
}
```

Listing 4.10: Implementation of the `n_approx_general` function

4.1.9 Assessment of the Accuracy of the Results

This section corresponds to step 5 and is final phase of our plan, where we carefully examine the accuracy of our methodology. As a primary test for the quality of the results, we aim to reproduce the curve of $\mathcal{D}_t^\gamma u$ on $[-t_\infty, t_\infty]$, and compare its shape with the original one from [3, page 12]. The newly computed curve is at the left and the former one at the right.



(a) Plot of the reconstructed $\mathcal{D}_t^\gamma u$ (b) Plot of the original $\mathcal{D}_t^\gamma u$

Figure 4.3: Plot of $\mathcal{D}_t^\gamma u$ for $0 < \gamma < 1$. As we ascend from the horizontal green line $\mathcal{D}_t^\gamma u\Big|_{\gamma=0}$, values of γ increase by 0.1 until we reach $\gamma = 0.9$, denoted by the pink curve. This is for $\text{sign}\left(\dfrac{dx_i}{d\sigma}\right) < 0$ and $p = 2$. The horizontal axis represents the range of t-values and the vertical axis the associated $\mathcal{D}_t^\gamma u$.

error	t
-4.744730e-008	3.6
-5.048329e-009	3.7
6.482569e-008	3.8
-4.435881e-009	3.9
2.060108e-007	4.0
-3.872901e-009	4.1
3.676208e-007	4.2
-3.364300e-009	4.3
-3.129406e-009	4.4
6.138696e-007	4.5
-2.703101e-009	4.6
7.505957e-007	4.7
-2.328432e-009	4.8
8.405479e-007	4.9
-2.001432e-009	5.0

Table 4.9: Error file for $\gamma = 0.7$

error	t
-1.784137e-010	3.6
-1.721758e-010	3.7
-1.664409e-010	3.8
-1.605218e-010	3.9
-1.547047e-010	4.0
-1.494032e-010	4.1
-1.443059e-010	4.2
-1.395319e-010	4.3
-1.351115e-010	4.4
-1.307046e-010	4.5
-1.269774e-010	4.6
-1.235263e-010	4.7
-1.206676e-010	4.8
-1.180839e-010	4.9
-1.161406e-010	5.0

Table 4.10: New error file for $\gamma = 0.7$

The reproduction of $\mathcal{D}_t^\gamma u$ was just the visual part of the assessment process. In fact, we still need to verify the precision of $\mathcal{D}_t^\gamma u$ values. To achieve this, we compute the absolute difference between $\mathcal{D}_t^\gamma u$ for $N = n$, $N = 2n$, and $p = 2$.

Initially, the `error` variable used in the stopping condition of the `writeFile` function was `error = abs(Simpson(lower, upper, n) - Simpson(lower, upper, n + 10))`. However, due to the non-monotonic and uncontrolled character of the errors' magnitude as depicted in Table 4.9, we adjusted the `error` variable to

```
error = abs(Simpson(lower, upper, n) - Simpson(lower, upper, 2*n)),
```

as mentioned in section 4.1.5. This modification yielded satisfactory results, as illustrated in

Table 4.10.

Implementation of $\mathcal{D}_t^\gamma u$ in C

Below is the implementation of the $\mathcal{D}_t^\gamma u$ function employed to reconstruct its curve .

Implementation of $\mathcal{D}_t^\gamma u$: The function `Du` calculates the value of $\mathcal{D}_t^\gamma u$ for $-5 \leq t \leq 5$.
Parameters list:

- `t`: the function's variable, between -5 and 5.
- `nt`: the number of subdivisions required to compute I_3.

Process:

- Calculate the first operand of $\mathcal{D}_t^\gamma u$ and store its value in `I1`.
- Calculate the second operand of $\mathcal{D}_t^\gamma u$ and store its value in `I2`.
- Calculate the third operand of $\mathcal{D}_t^\gamma u$, the one with the integral, and store its value in `I3`.

```c
double Du(double t, long int nt, double tmax, double p, double g) {

  double I1 = I_1(t, tmax, p, g);
  double I2 = I_2(t, tmax, p, g);
  double I3 = I_3(t, tmax, nt, p, g);

  return I1 + I2 - I3;

}
```

Listing 4.11: Implementation of the $\mathcal{D}_t^\gamma u$ function in C

Implementation of I_1, I_2, and I_3: I_1, I_2 and I_3 are used to implement respectively the first, second and third operands of $\mathcal{D}_t^\gamma u$ as defined in section 4.1.4.

```c
//Implementation of I_1

double I_1(double t, double tmax, double p, double g) {

  return (pow(tmax, -g) / (tgamma(1 - g))) * (u(t-tmax, p) - u(t, p));

}

//Implementation of I_2

```

```
double I_2(double t, double tmax, double p, double g) {

  return (pow(tmax, 1 - g) / tgamma(2 - g)) * (u1(t-tmax, p));

}

//Implementation of I_3

double I_3(double t, double tmax, long int nt, double p, double g) {

  return (1 / tgamma(2 - g)) * simpson(t, t-tmax, nt, p, g);

}
```

Listing 4.12: Implementation of I_1, I_2 and I_3 in C.

Chapter 5

Conclusion

Observations and Results

In this thesis, we have investigated the numerical approximation of the subdiffusive Gierer-Meinhardt model with controlled precision. Our research has yielded several key findings that contribute to our understanding of the model.

We began by defining and exploring the concepts of reaction-diffusion, elucidating the main difference between normal and anomalous diffusion: the rate at which particles spread across the reaction domain in each case. Specifically, during normal diffusion, the mean square displacement of particles can be expressed as a linear function of time, while in anomalous diffusion, this mean square displacement manifests as a fractional power of time.

Through our examination of integer and fractional calculus, we observed that certain rules and properties extend to fractional calculus, albeit with some limitations. For instance, the composition rule $d^q d^Q f = d^{q+Q} f$ extends to fractional calculus except in cases where $f \neq 0$ and $d^Q f = 0$. The term-by-term differentiation and integration of infinite series extend to fractional calculus under similar convergence conditions as classical calculus. This requires both the pointwise convergence of the series $\sum_{j=0}^{\infty} f_j$ and the uniform convergence of $\sum_{j=0}^{\infty} d^q f_j$ for term-by-term differentiation, and the uniform convergence of $\sum_{j=0}^{\infty} f_j$ for term-by-term integration over a specific interval. We found that while the scale change property, which proved to be highly beneficial when transitioning from the (x, t) axis to the (y_i, σ) axis, remains applicable in fractional calculus without specific restrictions, the chain rule does not extend due to the non-local nature of fractional derivatives or integrals.

Regarding the computation of the fractional operator of $\mathcal{D}_t^{\gamma}$, we observed that the lowest number of subdivisions required to achieve a controlled precision of 10^{-10} occurred for $p = 1.5$, $\gamma = 0.1$, and $t = 5$, totaling 17083 subdivisions. Conversely, the highest number of subdivisions exceeded 1 billion and occurred for $p = 4.5$, $\gamma = 0.9$, and $t = 0.1$. These results align with expectations, as the curve of of $\mathcal{D}_t^\gamma$ for the former case exhibited a nearly horizontal line around $t = 5$, while the latter showed a steep slope around $t = 0.1$.

Finally, in our verification process, a significant decision we made was to assess the achieved integration precision against the number of subdivisions returned by our program over a wider interval $[n, 2n]$ instead of focusing solely on close values such as n and $n + 10$, ensuring that of $\mathcal{D}_t^\gamma$ maintains consistent precision across a substantial range. The objective of calculating of $\mathcal{D}_t^\gamma$ numerically, with controlled precision, has therefore been achieved. This operator can therefore be used in system (3.23) to determine the values of $\frac{dx_i}{d\sigma}$ and $H(\sigma)$ with the desired precision.

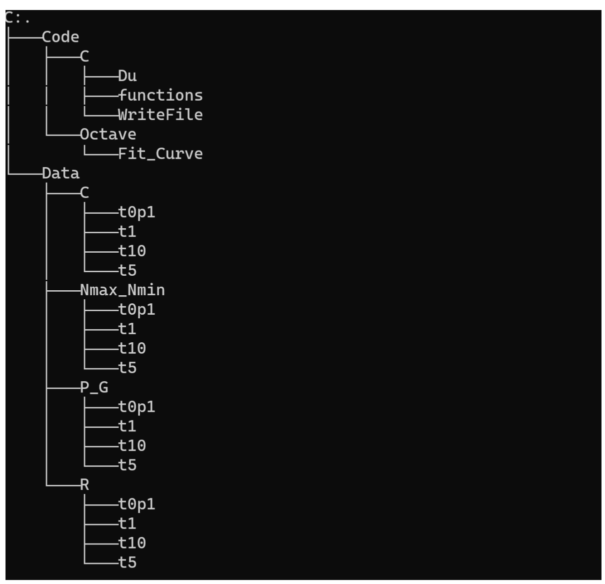
Appendices

Appendix A

Structure of the Project

Repository Tree

Below is the repository tree of the project. At the root of the project, you have two main repositories, Code and Data.



```
C:.
├───Code
│   ├───C
│   │   ├───Du
│   │   ├───functions
│   │   └───WriteFile
│   └───Octave
│       └───Fit_Curve
└───Data
    ├───C
    │   ├───t0p1
    │   ├───t1
    │   ├───t10
    │   └───t5
    ├───Nmax_Nmin
    │   ├───t0p1
    │   ├───t1
    │   ├───t10
    │   └───t5
    ├───P_G
    │   ├───t0p1
    │   ├───t1
    │   ├───t10
    │   └───t5
    └───R
        ├───t0p1
        ├───t1
        ├───t10
        └───t5
```

Figure A.1: Tree diagram of the project repository.

- Repository path: `\Code`.
- Repository description: Contains all the code for the project, either in C or in Octave.
- Repository content: `C`, `Octave`.

- Repository path: `\Code\C`.
- Repository description: Contains all the C code for the project.
- Repository content: `Du`, `functions`, `WriteFile`.
  * Repository path: `\Code\C\functions`.
  * Repository description: Contains all the functions and their prototypes used to approximate the number of subdivisions.
  * Repository content: `functions.h`, `functions.c`.
    · File name: `functions.h`.
    · Contains all the functions' prototypes used to approximate the number of subdivisions.

    · File name: `functions.c`.
    · File description: Contains the implementation of all the functions used in the approximation process.
    · File content: `sech`, `u`, `u1`, `u2`, `integrand`, `I_1`, `I_2`, `I_3`, `Du`, `simpson`, `findPosition_p`, `findPosition_g`, `linearN_T`, `bilinearN_p_g`, `n_approx`, `n_approx_general`, `N_T`, `N_logT`, `logN_T`, `logN_logT`, `even`, `reverse_n`, `join`.

    · File name: `functions.h`.
    · File description: Contains the prototypes of all the functions used in the approximation process.
  * Repository path: `\Code\C\Du`.
  * Repository description: Contains the C file used to reconstruct the curve of $\mathcal{D}_t^\gamma u$.
  * Repository content: `Du.c`.
    · File name: `Du.c`.
    · File description: Contains the code used to reconstruct the curve of $\mathcal{D}_t^\gamma u$.
  * Repository path: `\Code\C\WriteFile`.
  * Repository description: Contains the C file used to implement the composite Simpson method and to print its returned value in text files.
  * Repository content: `WriteFile.c`.
    · File name: `WriteFile.c`.
    · File description: Contains the C code used to implement the composite Simpson method and to print its returned value in text files.
- Repository path: `\Code\Octave`.
- Repository description: contains all the Octave code of the project.

- Repository content: `Fit_Curve`.
  - Repository path: `\Code\Octave\Fit_Curve`.
  - Repository description: Contains all the Octave files used to fit the residuals.
  - Repository content: `test1.m`, `fit_curve.m`, `fit_curvef.m`
    - file name: `test1.m`.
    - file description: Main file containing the overall logic of the fitting process.
    - file name: `fit_curve.m`.
    - file description: Contains the implementation of the `fit_curve` function which use is explained later in this document.
    - file name: `fit_curvef.m`.
    - file description: Contains the implementation of the `fit_curvef` function which use is explained later in this document.

- Repository path: `\Data`.
- Repository description: Contains all the data used in our project.
- Repository content: `P_G`, `Nmax_Nmin`, `R`, `C`.
  - Repository path: `\Data\P_G`.
  - Repository description: Holds the files containing the returned value of the Simpson method for $t = 0.1, 1, 5$.
  - Repository content: `t0p1`, `t1`, `t5`.

  - Repository path: `\Data\C`.
  - Repository description: Holds the files containing the $c(c_1, c_2)$ parameters for $t = 0.1, 1, 5$.
  - Repository content: `t0p1`, `t1`, `t5`.

  - Repository path: `\Data\Nmax_Nmin`.
  - Repository description: Holds the files containing the minimum and maximum number of subdivisions for $t = 0.1, 1, 5$.
  - Repository content: `t0p1`, `t1`, `t5`.

  - Repository path: `\Data\R`.
  - Repository description: Holds the files containing the residuals for $t = 0.1, 1, 5$.
  - Repository content: `t0p1`, `t1`, `t5`.

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