

A Grünwald–Letnikov scheme for fractional operators of Havriliak–Negami type

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Abstract: In this paper we propose the generalization of the Grünwald–Letnikov scheme to fractional differential operators of Havriliak–Negami type; these operators have important applications in the description and simulation of polarization processes in anomalous dielectrics with hereditary properties. We discuss in details the technique used for generalizing the proposed scheme, we provide a recursive relationship for the evaluation of the corresponding weights and we study some of their main properties.

Key–Words: Fractional calculus, Havriliak–Negami, Grünwald–Letnikov, convolution quadrature, dielectrics

1 Introduction

During the last decades, integral and differential operators of fractional (i.e., non–integer) order have been studied with an increasing interest motivated by the suitability in modeling systems exhibiting anomalous and/or memory preserving properties.

The theoretical analysis and the numerical approximation of fractional derivatives and fractional differential equations is therefore an active area of research with important applications in a wide range of fields such as biology, chemistry, engineering, finance, physics and so on.

More recently, the observation of experimental data has showed that in some systems the return to the equilibrium after the action of an external excitation obeys to some laws of fractional type (due to memory effects) but can not be described in a satisfactory way by means of standard operators of fractional order; it is therefore necessary to introduce and study more sophisticated operators. This is the case of the relaxation of Havriliak–Negami type [9] used to describe polarization processes in media with anomalous dielectric properties.

Havriliak–Negami models are usually derived in the Fourier or Laplace transform domain but for their simulation in the time–domain some completely new operators (based on fractional differentiation) are involved. These operators are much more complicated than classical fractional derivatives and their use for simulation purposes is still a challenge since very few approaches have been so far studied for their approximation.

For this reason, an important task, which motivates the present work, is the development of ad–hoc numerical techniques in order to simulate, in the time–domain, Havriliak–Negami models.

In this paper we consider a classical and widely used scheme for approximating derivatives and integrals of fractional order, namely the Grünwald–Letnikov scheme, and we discuss an approach for the generalization to operators of Havriliak–Negami type. A recursive relation for the evaluation of the weights in the resulting scheme is presented and the main properties of the weights are also investigated.

This work is organized as follows. In Section 2 we review some basic facts concerning derivatives and integrals of fractional order and in Section 3 we present the Grünwald–Letnikov operators and the corresponding approximated schemes. Section 4 is devoted to the description of Havriliak–Negami operators. We hence present, in Section 5, an alternative approach for deriving the Grünwald–Letnikov scheme for fractional integral and derivatives thanks to which we are able to generalize such scheme to operators of Havriliak–Negami type and study some of its main properties. Finally, we present some concluding remarks in Section 6.

2 Derivatives and integrals of fractional order

Several operators have been proposed throughout the years to define derivatives of non–integer order. Al-

though the Riemann–Liouville definition is perhaps the most important from the historical and the theoretical point of view, for practical applications the definition named after the Italian scientist Francesco Caputo is usually preferred since it allows to take into account initial conditions expressed in terms of easily measurable physical quantities.

We refer to any of the classical textbook on fractional calculus [3, 24, 25] for a review of the main properties of the different operators.

For any real $\alpha > 0$, and denoted with $m = \lceil \alpha \rceil$ the smallest integer such that $m > \alpha$, the Caputo’s derivative of fractional order α is defined according to

$${}_0D_t^\alpha y(t) = \frac{1}{\Gamma(m - \alpha)} \int_0^t \frac{y^{(m)}(\tau)}{(t - \tau)^{\alpha+1-m}} d\tau,$$

where with $y^{(m)}$ we indicate the classical derivative of integer order m (the function y is assumed to have absolutely continuous derivative of order $m - 1$ on some interval $[0, T]$).

The above fractional derivative is strictly related to the Riemann–Liouville (RL) integral of non integer order $\alpha > 0$

$${}_0I_t^\alpha y(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} y(\tau) d\tau.$$

Indeed, given the functional equation

$${}_0D_t^\alpha y(t) = g(t),$$

it is possible to express $y(t)$ in terms of the RL integral of $g(t)$ as

$$y(t) = Y_{m-1}(t) + {}_0I_t^\alpha g(t),$$

where $Y_{m-1}(t)$ is the Taylor polynomial, centered at the origin, of degree $m - 1$ for the function $y(t)$

$$Y_{m-1}(t) = \sum_{k=0}^{m-1} \frac{t^k}{k!} y^{(k)}(0).$$

Equivalently, $g(t)$ can be reformulated in terms of the RL integral (of negative and non integer order $-\alpha$) of $y(t)$ as

$$g(t) = {}_0I_t^{-\alpha} (y(t) - Y_{m-1}(t)),$$

where, due to the presence of the singularity of order $\alpha + 1$, the integral must be intended as an Hadamard’s finite–part integral. Obviously, to guarantee the uniqueness it is necessary to assign a set of initial conditions

$$y^{(k)}(0) = y_{0,k}, \quad k = 0, 1, \dots, m - 1.$$

3 Grünwald–Letnikov operators

An alternative approach to define, and at the same time approximate, derivatives of fractional order is given by the Grünwald–Letnikov (GL) operators.

GL operators are based on a classical concept in traditional calculus for which derivatives of integer order can be represented as limits of finite differences.

Indeed, under the assumption $y \in \mathcal{C}^m([0, T])$, $m \in \mathbb{N}$, it is well–known that the m –order derivative of y at $t \in (0, T]$ can be obtained as

$$D^m y(t) = \lim_{h \rightarrow 0} \frac{1}{h^m} \sum_{k=0}^m (-1)^k \binom{m}{k} y(t - kh), \quad (1)$$

where, as usual, the binomial coefficients are defined according to

$$\binom{m}{k} = \frac{m(m-1) \cdots (m-k+1)}{k!} = \frac{m!}{k!(m-k)!}.$$

Binomial coefficients can be generalized to real arguments by means of the Euler’s gamma function

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

for which it is a well–known result that $\Gamma(1) = 1$ and $\Gamma(z + 1) = z\Gamma(z)$, for any $z > 0$. Since for $m \in \mathbb{N}$ it is $\Gamma(m + 1) = m!$, the gamma function can be considered as the generalization of the factorial to real arguments and replacing m with any real positive α in the formula for the binomial coefficients leads to

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

Since the relation $\Gamma(z + 1) = z\Gamma(z)$ allows to extend the gamma function also for $z < 0$ when $z \notin \{0, -1, -2, -3, \dots\}$ (see [11]), the above formula for the binomial coefficients can be applied also to $\alpha < 0$ with $\alpha \notin \{0, -1, -2, -3, \dots\}$.

For $y \in \mathcal{C}^m([0, T])$, $m = \lceil \alpha \rceil$, it is therefore possible to extend (1) to the fractional order $\alpha > 0$ by means of

$${}_0\bar{D}_t^\alpha y(t) = \lim_{N \rightarrow \infty} \frac{1}{h^\alpha} \sum_{k=0}^N \omega_k^{(\alpha)} y(t - kh) \quad (3)$$

for $t \in (0, T]$ and where h depends on t and N according to $h = t/N$. Here $y(t)$ is continued to the left of the origin by assuming $y(t) = 0$ for $t < 0$ and, for shortness, we denote with $\omega_k^{(\alpha)}$ the weights

$$\omega_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}.$$

The operator ${}_0\bar{D}_t^\alpha$ is known as the differential Grünwald–Letnikov (GL) operator, after the mathematicians Grünwald [8] and Letnikov [12] who introduced, for $y \in \mathcal{C}([0, T])$ and $t \in (0, T]$, its integral counterpart

$${}_0\bar{I}_t^\alpha y(t) = \lim_{N \rightarrow \infty} h^\alpha \sum_{k=0}^N \omega_k^{(-\alpha)} y(t - kh). \quad (4)$$

The importance of differential and integral GL operators is not only for historical and theoretical purposes but also for practical applications. Indeed, it is possible to truncate the infinite series in (3) and (4) in order to provide an approximation of the respective operators, as for instance for

$${}_0\bar{I}_t^\alpha y(t_n) \approx h^\alpha \sum_{k=0}^n \omega_{n-k}^{(-\alpha)} y(t_k), \quad (5)$$

where $t_k = kh$.

Since the well-known equivalence (see, for instance, [3]) ${}_0D_t^\alpha y(t) = {}_0\bar{D}_t^\alpha (y(t) - Y_{m-1}(t))$, which allows to reformulate the Caputo’s derivative in terms of the GL operator, it is possible to provide an approximation of the Caputo’s derivative by means of

$${}_0D_t^\alpha y(t_n) \approx \frac{1}{h^\alpha} \sum_{k=0}^n \omega_{n-k}^{(\alpha)} [y_k - Y_{m-1}(t_k)]. \quad (6)$$

For a review of the main properties of the GL operators, and of the corresponding approximated GL schemes, we refer, for instance, to [3, 6, 7, 25].

The weights $\omega_n^{(\alpha)}$ of the GL scheme satisfies some important properties. They can be equivalently formulated as [23]

$$\omega_n^{(\alpha)} = \binom{n - \alpha - 1}{n} = \frac{\Gamma(n - \alpha)}{\Gamma(-\alpha)\Gamma(n + 1)}$$

and it is immediate to see that they can be evaluated in a recursive way according to

$$\omega_0^{(\alpha)} = 1, \quad \omega_n^{(\alpha)} = \left(1 - \frac{\alpha + 1}{n}\right) \omega_{n-1}^{(\alpha)}. \quad (7)$$

For a proof of the following properties of the weights $\omega_n^{(\alpha)}$ and $\omega_n^{(-\alpha)}$ we refer to one of the aforementioned references.

Proposition 1. *For any real α and $0 < \xi < 1$ it is*

$$\sum_{n=0}^{\infty} \omega_n^{(\alpha)} \xi^n = (1 - \xi)^\alpha$$

and, moreover, the above series converges also when $\xi = 1$ and $\alpha \geq 0$.

Proposition 2. *Let $0 < \alpha < 1$. Then*

1. $\omega_0^{(\alpha)} = 1$ and $\omega_n^{(\alpha)} \leq 0$ for any $n \geq 1$;
2. $|\omega_{n+1}^{(\alpha)}| < |\omega_n^{(\alpha)}| < \omega_0^{(\alpha)}$, $n \geq 1$;
3. $\lim_{n \rightarrow \infty} \sum_{n=0}^{\infty} \omega_n^{(\alpha)} = 0$.

Proposition 3. *Let $-1 < \alpha < 0$. Then*

1. $\omega_0^{(\alpha)} = 1$ and $\omega_n^{(\alpha)} \geq 0$ for any $n \geq 1$;
2. $\omega_{n+1}^{(\alpha)} < \omega_n^{(\alpha)} < \omega_0^{(\alpha)}$, $n \geq 1$;
3. $\lim_{n \rightarrow \infty} \sum_{n=0}^{\infty} \omega_n^{(\alpha)} = +\infty$.

4 Fractional operators of Havriliak–Negami type

The polarization processes in anomalous dielectrics, and the corresponding relaxation laws, are usually investigated in the Fourier or Laplace transform domain where the relationship between the external excitation $g(t)$ and the response $y(t)$ of the media is expressed by means of a characteristic function. In particular, in the Laplace transform domain, we assume the relationship

$$Y(s) = H(s) * G(s) \quad (8)$$

where $s \in \mathbb{C}$, G and Y are the Laplace transform of the external excitation g and the response y respectively and $H(s)$ is the transfer function.

In models based only on classical derivatives of integer order (models of Debye type) $H(s)$ is usually a rational function of the type

$$H(s) = \frac{1}{s + \lambda},$$

while in models based on fractional differential equations (also referred to as Cole–Cole models) a transfer function with real powers

$$H(s) = \frac{1}{s^\alpha + \lambda}$$

is instead involved.

In the Havriliak–Negami models the transfer function generalizes the Debye and Cole–Cole models by incorporating a further parameter γ

$$H(s) = \frac{1}{(s^\alpha + \lambda)^\gamma}, \quad (9)$$

where $0 < \alpha \leq 1$ and λ is any positive real value. Although in most papers γ is restricted to the interval $(0, 1]$, it has been recently proved [2, 19] that for the physical feasibility of the model the condition on γ can be relaxed to $0 < \gamma \leq 1/\alpha$, thus allowing a wider range of coefficients.

Since $H(s)$ is a multivalued function with a branch point in the origin, in order to make it single-valued we consider a branch cut along the negative real half-axis. The function $H(s)$ is hence analytical on $\mathbb{C} \setminus \mathbb{R}^-$.

Unfortunately, the representation in the time-domain of the Havriliak–Negami relaxation is not immediate and simple. Several authors represent the corresponding in the time-domain of (8-9) by means of a fractional pseudo-differential operator

$$y(t) = (\lambda + {}_0D_t^\alpha)^\gamma g(t)$$

which, however, can be considered just as a symbol since the formal definition of $(\lambda + {}_0D_t^\alpha)^\gamma$ is not clear.

A first formalization of the differential operator $(\lambda + {}_0D_t^\alpha)^\gamma$ was proposed by Nigmatullin and Ryabov [21] who derived a combination of exponential and classical fractional derivative operators

$$(\lambda + {}_0D_t^\alpha)^\gamma = {}_0\mathcal{F}_t^\alpha[-\lambda] {}_0D_t^{\alpha\gamma} {}_0\mathcal{F}_t^\alpha[\lambda],$$

where

$${}_0\mathcal{F}_t^\alpha[\lambda] = \exp\left(\frac{\lambda t}{\alpha} {}_0D_t^{1-\alpha}\right).$$

Despite the extremely elegant framework in which the above representation of $(\lambda + {}_0D_t^\alpha)^\gamma$ has been derived, its use for practical computation is not easy since evaluating or approximating the exponential ${}_0\mathcal{F}_t^\alpha[\pm\lambda]$ of fractional derivative operators is a very complicate task.

More recently, it has been proposed in [22] to expand $(\lambda + {}_0D_t^\alpha)^\gamma$ in terms of an infinite series of derivative operators of fractional order as

$$(\lambda + {}_0D_t^\alpha)^\gamma = \sum_{k=0}^{\infty} \binom{\gamma}{k} \lambda^k {}_0D_t^{\alpha(\gamma-k)},$$

where the extension of the binomial coefficient to real arguments is the same presented in (2).

From an applicative point of view it is possible to use this approach in computation by truncating the infinite series as proposed in [1, 20]. Anyway, the number of terms which must be considered in the truncated series depends on the characteristic parameters α , γ and λ and it is quite difficult to determine this number in order to obtain a desired accuracy, for the final approximation, in the time-domain.

These non negligible issues justify the investigation of ad-hoc techniques for the numerical approximation of $(\lambda + {}_0D_t^\alpha)^\gamma$.

5 Grünwald–Letnikov schemes for Havriliak–Negami operators

5.1 Convolution quadrature rules

The GL fractional operators (3) and (4) has been intensively studied by several authors. Moreover, for several time, a formal proof of the convergence properties of the GL schemes (5) and (6) has not been provided until the work of Lubich who presented, in a series of influential papers [13, 14, 15], an elegant and accurate framework for deriving and studying convolution quadrature rules.

Given an equispaced grid $t_n = nh$, with step-size $h > 0$, a numerical approximation for the convolution integral

$$y(t) = \int_0^t f(t - \tau)g(\tau) d\tau$$

can be obtained by means of a discrete convolution

$$y_n = \sum_{j=0}^n \omega_{n-j}g(t_j) \tag{10}$$

which generalizes some classical numerical method for ordinary differential equations (ODEs) and with the convolution weights ω_n depending on the step-size h , on the kernel f and on the underlying method for ODEs.

In particular, let us consider the initial value problem for the ODE

$$y'(t) = g(t, y(t)), \quad y(0) = y_0,$$

and a k -step linear multistep method (LMM)

$$\sum_{j=0}^k \alpha_j y_{n+j-k} = h \sum_{j=0}^k \beta_j y_{n+j-k}$$

with $\rho(\xi) = \alpha_0\xi^k + \dots + \alpha_{k-1}\xi + \alpha_k$ and $\sigma(\xi) = \beta_0\xi^k + \dots + \beta_{k-1}\xi + \beta_k$ respectively the first and second characteristic polynomial. Denoted with

$$\delta(\xi) = \frac{\rho(\xi)}{\sigma(\xi)}$$

the generating function of the LMM, the weights ω_n are obtained as the coefficients in the power series

$$F\left(\frac{\delta(\xi)}{h}\right) = \sum_{n=0}^{\infty} \omega_n \xi^n,$$

where F is the Laplace transform of the kernel f .

In order to properly work, two main conditions need to be satisfied:

H1: outside a sector with an acute angle to the negative real axis the Laplace transform $F(s)$ must be analytic and satisfy $|F(s)| \leq M|s|^\mu$ for some constant $M < \infty$ and $\mu > 0$;

H2: the underlying LMM method must be consistent, strong stable and its stability region must include the sector introduced in the assumption **H1**.

Under the above assumptions it is possible to prove the convergence of the convolution quadrature (10). In particular, for first order methods the following result [14, Theorem 3.1] holds.

Theorem 4. *Let $g \in C^1([0, T])$. If the underlying LMM method is convergent of the first order, then*

$$|y(t_n) - y_n| \leq Ct^{\mu-1}h(|g(0)| + t_n \max_{0 \leq t \leq t_n} |g'(t)|)$$

for a constant C independent of h .

Approximations with higher order of convergence are obtained after adding in (10) a starting term in order to deal with the possibly singular behavior of $y(t)$ close to the origin.

On of the most simple methods for solving an ODE is the backward Euler method

$$y_n = y_{n-1} + hg(t_n, y_n)$$

for which the quotient of the generating polynomials is clearly

$$\delta(\xi) = (1 - \xi)$$

and satisfies the above assumption **H2**.

Since the RL integral ${}_0I_t^\alpha$ is a convolution integral, with kernel $t^{\alpha-1}/\Gamma(\alpha)$ whose Laplace transform is $s^{-\alpha}$, it is possible to generate a convolution quadrature approximating ${}_0I_t^\alpha$ and generalizing the backward Euler method by using as convolution weights the coefficients in the power series of

$$\left(\frac{1 - \xi}{h}\right)^{-\alpha} = h^\alpha(1 - \xi)^{-\alpha}.$$

Thanks to Proposition 1, it is easy to observe that the method developed in this way corresponds exactly to the GL scheme (5) and, since Theorem 4 holds, the first order of convergence of the GL scheme can be inferred.

5.2 Application to HN

The convolution quadratures devised by Lubich can be extended to operators of Havriliak–Negami type.

To this purpose we first observe that $H(s)$ satisfies the assumption **H1**; moreover, we can reformulate (8) in the time–domain as

$$y(t) = \int_0^t h(t - \tau)g(\tau) d\tau,$$

where $h(t)$ is the inverse Laplace transform of $H(s)$.

It is well–known that $h(t)$ can be expressed in terms of a 3–parameters Mittag–Leffler (ML) function [2], also known as the Prabhakar function, generalizing the classical 1 and 2 parameters ML functions which play a fundamental role in fractional calculus (see, for instance, [5, 16, 17, 18]).

For simplicity we assumed initial conditions equal to zero although the identification of suitable initial conditions for problems of this type is a topic which deserves a more in–depth investigation.

In order to derive a convolution quadrature based on the backward Euler method, i.e. $\delta(\xi) = 1 - \xi$, generalizing the GL scheme (5) to Havriliak–Negami operators, we must consider the following generating function

$$H\left(\frac{\delta(\xi)}{h}\right) = \frac{1}{\left(\frac{(1 - \xi)^\alpha}{h^\alpha} + \lambda\right)^\gamma}$$

which, after putting

$$H_{\alpha,\gamma}(\xi; z) = \left(\frac{(1 - \xi)^\alpha + z}{1 + z}\right)^{-\gamma},$$

can be written as

$$H\left(\frac{\delta(\xi)}{h}\right) = \Phi_{\alpha,\gamma}(h; \lambda)H_{\alpha,\gamma}(\xi; h^\alpha\lambda),$$

where $\Phi_{\alpha,\gamma}(h; \lambda)$ depends on the characteristic parameters α , γ and λ and on the step–size h , and it is given by

$$\Phi_{\alpha,\gamma}(h; \lambda) = h^{\alpha\gamma}(1 + h^\alpha\lambda)^{-\gamma}.$$

We can therefore consider the convolution quadrature

$$y_n = \Phi_{\alpha,\gamma}(h; \lambda) \sum_{k=0}^n \tilde{\omega}_{n-k} g(t_k) \tag{11}$$

where now the weights $\tilde{\omega}_n$ are the coefficients in the power expansion of $H_{\alpha,\gamma}(\xi; h^\alpha\lambda)$, i.e.

$$H_{\alpha,\gamma}(\xi; h^\alpha\lambda) = \sum_{n=0}^{\infty} \tilde{\omega}_n \xi^n.$$

It is elementary to see that when $\lambda = 0$ and $\gamma = 1$ it is $\Phi_{\alpha,\gamma}(h; \lambda) = h^\alpha$ and $H_{\alpha,\gamma}(\xi; h^\alpha \lambda) = (1 - \xi)^{-\alpha}$ and hence the GL scheme (5) for approximating ${}_0\bar{I}_t^\alpha$ is obtained.

To evaluate the convolution weights it was proposed in [15] the use of the representation of each coefficient by means of the Cauchy integral and hence its approximation on a circular contour around the origin by means of the trapezoidal rule.

An alternative approach based on the Miller's formula was instead presented in [4]. The Miller's formula [10, Theorem 1.6c] is an efficient tool for evaluating, in a recursive way, the coefficients of a formal power series (FPS) raised to any power and it is based on the following result.

Theorem 5. Let $\varphi(\xi) = 1 + \sum_{n=1}^\infty a_n \xi^n$ be a FPS. Then for any $\beta \in \mathbb{C}$,

$$(\varphi(\xi))^\beta = \sum_{n=0}^\infty v_n^{(\beta)} \xi^n,$$

where coefficients $v_n^{(\beta)}$ are recursively evaluated as

$$v_0^{(\beta)} = 1, \quad v_n^{(\beta)} = \sum_{j=1}^n \left(\frac{(\beta+1)j}{n} - 1 \right) a_j v_{n-j}^{(\beta)}.$$

One of the simplest case of application of the Miller's formula is in the generation of the coefficients of the GL scheme, by applying it to the FPS $(1-\xi)^\alpha$ and hence obtaining the recursive relationship (7) which allows the evaluation of the first N weights $\omega_n^{(\alpha)}$, $n = 0, \dots, N-1$ with a computational cost proportional to N .

The computation of the convolution weights in the FPS of $H_{\alpha,\gamma}(\xi; h^\alpha \lambda)$ is performed in two steps.

The coefficients in the expansion of $(1-\xi)^\alpha$ are first evaluated by means of the recurrence (7). Hence, since $\omega_0^{(\alpha)} = 1$, the function $H_{\alpha,\gamma}(\xi; h^\alpha \lambda)$ is rewritten as

$$\begin{aligned} H_{\alpha,\gamma}(\xi; h^\alpha \lambda) &= \left(\frac{1 + \sum_{n=1}^\infty \omega_n^{(\alpha)} \xi^n + h^\alpha \lambda}{1 + h^\alpha \lambda} \right)^{-\gamma} \\ &= \left(1 + \sum_{n=1}^\infty \frac{\omega_n^{(\alpha)}}{1 + h^\alpha \lambda} \xi^n \right)^{-\gamma} \end{aligned}$$

and the Miller's formula of Theorem 5 is applied to the above FPS with negative power $-\gamma$; the resulting recursive relationship for $\tilde{\omega}_n$ is therefore

$$\tilde{\omega}_n = \sum_{j=1}^n \left(\frac{(1-\gamma)j}{n} - 1 \right) \frac{\omega_j^{(\alpha)}}{1 + h^\alpha \lambda} \tilde{\omega}_{n-j}, \quad (12)$$

with $\tilde{\omega}_0 = 1$, and the overall computational cost for the first N weights is proportional to N^2 .

We are able to prove that the weights $\tilde{\omega}_n$ of the convolution quadrature (11) satisfy the following properties.

Proposition 6. Let $0 < \alpha < 1$, $\lambda > 0$ and $\gamma > 0$. Then

1. $\tilde{\omega}_0 = 1$ and $\tilde{\omega}_n > 0$ for $n \geq 1$;

2.
$$\sum_{n=0}^\infty \tilde{\omega}_n = \left(\frac{1 + h^\alpha \lambda}{h^\alpha \lambda} \right)^\gamma$$

Proof: The first part of point 1. is obvious; for the second part we first observe that $1 + h^\alpha \lambda > 0$ and $\omega_j^{(\alpha)} < 0$, for $j \geq 1$, thanks to Proposition 2. Thus the proof follows from (12) by induction on n since for $\gamma > 0$ it is

$$\frac{(1-\gamma)j}{n} - 1 \leq 0, \quad j = 1, \dots, n.$$

For point 2. we observe that

$$\begin{aligned} \sum_{n=0}^\infty \tilde{\omega}_n &= \tilde{H}_{\alpha,\gamma}(\xi; h^\alpha \lambda) \Big|_{\xi=1} = \\ &= \left(1 + \frac{(1-\xi)^\alpha - 1}{1 + h^\alpha \lambda} \right)^{-\gamma} \Big|_{\xi=1} \end{aligned}$$

and hence the proof easily follows. \square

6 Conclusion

In this paper, based on the work of Lubich [14, 15], the Grünwald–Letnikov scheme has been generalized to the Havriliak–Negami model, see Equation (11), and the recurrence relation (12) has been provided for the computation of the weights. Some of the properties of the weights in the new scheme of Grünwald–Letnikov type have been investigated in Proposition 6.

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