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Grünwald–Letnikov operators for fractional relaxation in Havriliak–Negami models☆

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ABSTRACT

Several classes of differential and integral operators of non integer order have been proposed in the past to model systems exhibiting anomalous and hereditary properties. A wide range of complex and heterogeneous systems are described in terms of laws of Havriliak–Negami type involving a special fractional relaxation whose behavior in the time-domain can not be represented by any of the existing operators. In this work we introduce new integral and differential operators for the description of Havriliak–Negami models in the time-domain. In particular we propose a formulation of Grünwald–Letnikov type which turns out to be effective not only to provide a theoretical characterization of the operators associated to Havriliak–Negami systems but also for computational purposes. We study some properties of the new operators and, by means of some numerical experiments, we present their use in practical computation and we show the superiority with respect to the few other approaches previously proposed in literature.

1. Introduction

Integral and differential operators of non integer order attract ever growing interest motivated by the large extent of applications in which they are fruitfully employed; models based on fractional integrals or fractional derivatives are indeed effective to describe complex phenomena in a variety of fields ranging from biochemistry to control theory, engineering, mechanics, physics and so on.

Alongside Riemann–Liouville operators, which are the basis of the fractional calculus, new specific fractional operators (e.g., of Caputo, Erdélyi–Kober, Marchaud, Riesz and Weyl type [1–4]) have been introduced with the aim of describing, in the most appropriate way, systems and models for which traditional operators are not sufficiently satisfactory.

New operators are usually proposed on the basis of theoretical considerations but in same cases specific operators are introduced from experimental observations after measuring, in the frequency domain, the response of a system to some external excitations and matching the experimental data to a theoretical model.

For several years only very simple models have been considered and the Debye model [5] has been the most popular because of the possibility of describing the corresponding action in the time domain by means of ordinary differential equations.

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Experimental observations on the asymmetry and broadness of the dielectric dispersion in some polymers [6] led, in 1967, to the formulation of the Havriliak–Negami (HN) model which is obtained by inserting two independent real powers in the classical Debye model.

Empirical laws of HN type, which are recognized as manifestation of simultaneous nonlocality and nonlinearity [7,8] in the response of disordered materials and heterogeneous systems, are nowadays applied in physics [9,10], in mechanical engineering [11], in the analysis of electric circuits [12] and, in particular, to describe dielectrics properties of dispersive and disordered media [13–15].

A major issue with the HN model, which has so far mainly studied in the frequency domain, is the absence of a formal representation in the time domain. Some noticeable efforts have been made to formulate new operators as combination of classic fractional derivatives [16–18] or to introduce specific convolution operators [19–21] (see also [22] for applications in fractional Poisson processes). Anyway, as a consequence of the non-linearity in the frequency domain, the corresponding integral and differential operators in the time domain are still not completely known in an explicit way [23].

The aim of this work is to contribute to fill this gap by introducing and investigating new integral and differential operators for the description of HN models in the time domain. In particular, we propose an approach based on fractional differences [24] which can be considered as the natural generalization of Grünwald–Letnikov (GL) operators, a class of operators widely used in fractional calculus.

The importance of GL operators is not only for historical and theoretical reasons but it is also related to the possibility of direct application in numerical computation since, in a straightforward way, they also provide a discretization scheme. The generalization to HN models is done on the basis of the work of Lubich [25,26] on quadrature rules for convolution integrals.

This paper is organized as follows. In Section 2 we review some basic definitions and properties and in Section 3, after introducing the HN model, we discuss the problem of its formulation in the time-domain in terms of fractional operators. We hence derive, in Section 4, integrals and derivatives of GL type for operators of HN type and we study some of their main properties. Numerical experiments are presented in Section 5 and some final remarks conclude the paper.

2. Integrals and derivatives of fractional order

Several types of integral and differential operators of non-integer order have been proposed and investigated in the past. From an historical point of view, the origins of the fractional calculus are strictly related to the *Riemann–Liouville* (RL) integral of real order $\alpha > 0$

$$J_{t_0}^{\alpha} y(t) = \frac{1}{\Gamma(\alpha)} \int_{t_0}^{t} (t-u)^{\alpha-1} y(u) du, \quad t \in [t_0, T], \tag{1}$$

where $\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t} dt$ is the Euler gamma function and $y \in L^1([t_0, T])$. We refer to the reviews [27,28] for historical notes on fractional calculus and to [29–33] for introductory material.

The left-inverse of the fractional integral (1) is the RL fractional derivative

$$D_{t_0}^{\alpha} y(t) \equiv D^m J_{t_0}^{m-\alpha} y(t) = \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dt^m} \int_{t_0}^{t} (t-u)^{m-\alpha-1} y(u) du,$$

where $m = \lceil \alpha \rceil$ is the smallest integer such that $m > \alpha$ and D^m and d^m/dt^m denote standard derivatives of integer order; the absolute continuity of y is required for the existence of $D_{t_0}^{\alpha} y(t)$ [29].

Some other fractional operators have been introduced for practical reasons or for describing specific phenomena in a more detailed way. For instance, the *Caputo* derivative, which allows to couple fractional differential equations with standard initial conditions of Cauchy type is defined, for m-times absolutely continuous functions, as

$${}^{C}D_{t_0}^{\alpha} y(t) \equiv J_{t_0}^{m-\alpha} D^m y(t) = \frac{1}{\Gamma(m-\alpha)} \int_{t_0}^{t} (t-u)^{m-\alpha-1} y^{(m)}(u) du$$

and it is strictly related to the RL derivative by means of the relationship

$${}^{C}D_{t_0}^{\alpha} y(t) = D_{t_0}^{\alpha} \left(y(t) - \sum_{k=0}^{m-1} \frac{(t-t_0)^k}{k!} y^{(k)}(t_0) \right). \tag{2}$$

Alternative definitions of integral and derivatives of fractional order are provided by means of GL operators which are based on the classic representation of the integer order derivative D^m as the limit of finite differences

$$D^m y(t) = \lim_{h \to 0} \frac{1}{h^m} \sum_{k=0}^{m} (-1)^k \binom{m}{k} y(t-kh), \quad t \in (t_0, T], \tag{3}$$

where, as usual, the binomial coefficients are

$$\binom{m}{k} = \frac{m(m-1)\cdots(m-k+1)}{k!} = \frac{m!}{k!(m-k)!}. \tag{4}$$