Theory and Numerical Approximations of Fractional Integrals and Derivatives

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Preface

Fractional calculus, which has two main features—singularity and nonlocality from its origin—means integration and differentiation of any positive real order or even complex order. It has a history of at least three hundred years, since it can be traced back to a letter from Gottfried Wilhelm Leibniz to Guillaume de l'Hôpital, dated 30 September 1695, in which the meaning of the one-half order derivative was first discussed and some remarks about its possibility were made. It is generally accepted that fractional calculus underwent two stages: from its beginning to the 1970s, and after the 1970s. At the first stage, fractional calculus was studied mainly by mathematicians as an abstract field containing only pure mathematical manipulations of little or no use. At the second stage, the paradigm began to shift from pure mathematical research to applications in various realms, such as anomalous diffusion, anomalous convection, power laws, allometric scaling laws, history dependence, long-range interactions, and so on.

Although numerical methods for fractional integrals and fractional derivatives have been collected and remarked in two review articles (Int. J. Bifurcation Chaos, 22 (4), 1230014, 2012; Int. J. Comput. Math., 95 (6-7), 1048–1099, 2018), and Chapter 2 of the book *Numerical Methods for Fractional Calculus* (CRC Press, Boca Raton, 2015), novel algorithms keep emerging and are widely scattered through many technical and scientific journals. A comprehensive book is required to collect and summarize the recent advances in numerical fractional calculus as well as the traditional and also most used algorithms.

This book aims at collecting and sorting out these studies, and includes two parts. One is about the background and theory of fractional calculus, which are presented in Chapters 1 and 2. The other is the major element of this book focusing on numerical approximations to fractional integrals and fractional derivatives, from Chapter 3 to Chapter 7.

In the first chapter, background and theory of fractional integrals are covered. Starting with introducing the Riemann-Liouville integral out of the description of the fractional diffusion equation, Chapter 1 conveys to the reader comprehensive knowledge on fractional integrals, by virtue of asymptotical derivation of anomalous diffusion and nonexponential relaxation patterns from basic random walk models and a generalized master equation. As a kind of frequently utilized fractional integral, the Riemann-Liouville integral is the protagonist of this chapter. The definition, existence conditions, and main properties, especially its relationship with the integer-order integral, are introduced. They are complementary instruments for theoretical analysis of fractional differential systems. Fractional integrals of some other types are also presented, along with the corresponding basic knowledge. What follows is fundamental knowledge on fractional derivatives presented in the coming chapter.

In Chapter 2, heavily utilized fractional derivatives (Riemann-Liouville derivative, Caputo derivative, Riesz derivative, and fractional Laplacian) are introduced. Some other well-known fractional derivatives are also mentioned. Definitions and properties of these fractional derivatives are routinely presented, as well as their correlations. These aspects are considered and the results help the reader in understanding fractional derivative operators as pseudo-differential operators, together with their tremendous application potential in applied science and engineering, not merely mathematical generalizations of the classical derivative operators. As an adequate tool describing unusual diffusion processes due to random displacements and Lévy flights, the fractional Laplacian is especially mentioned. The relationship between the fractional Laplacian and Riesz derivative is clarified in detail, elucidating that the fractional Laplacian seems to possess a larger range of applications in characterizing anomalous diffusion and anomalous convection, which can be seen from the fact that the fractional Laplacian has attracted increasing interest. The Riesz derivative seems to be neglected. If one carefully and meticulously reads the encyclopedic book *Fractional Integrals and Derivatives: Theory and Applications* (Gordon and Breach Science Publishers, Amsterdam, 1993), he/she may find its usefulness, profoundness, and beauty. In effect, the Riesz derivative defined on $\mathbb{R}$ is essentially the fractional Laplacian defined on $\mathbb{R}$. And the fractional Laplace operator is also known as the Riesz fractional derivative operator (Fract. Calc. Appl. Anal., 20 (1), 7–51, 2017). The partial Riesz derivative in multiple dimensions seems inconvenient for applications. The fractional Laplacian in the multi-dimensional case is therefore adopted. An alternative definition of the fractional Laplacian, i.e., the so-called spectral definition, is a simple generalization of a positive definite operator in finite dimensions (i.e., the symmetric and positive definite matrix in finite dimensional linear space). This spectral definition is different from the aforementioned fractional Laplacian in the sense of Riesz.

On the other hand, different from integer order derivative, semigroup properties for fractional derivatives generally do not hold. The equalities

$$\sin^{(\alpha)}(x) = \sin\left(x + \frac{\pi\alpha}{2}\right) \tag{1}$$

and

$$\cos^{(\alpha)}(x) = \cos\left(x + \frac{\pi\alpha}{2}\right) \tag{2}$$

generally do not hold either when the derivative order α is not a positive integer. Definite conditions for fractional differential equations are also carefully described. These three aspects have often been misused and so are highlighted in Chapter 2.

Once acquainted with fractional calculus, it remains to study fractional differential equations. The reality is that most fractional differential equations are difficult or even impossible to analytically solve. Consequently, numerical solving fractional differential equations becomes a preferred alternative. And there is no doubt that techniques evaluating fractional integrals and fractional derivatives are fundamental in this regard. Part II collects and presents almost all the existing numerical approximations to fractional integrals and fractional derivatives. Numerical approximations to fractional integrals, the Caputo derivative, Riemann-Liouville derivative, Riesz derivative, and fractional Laplacian are included in Chapters 3–7, respectively.

Riemann-Liouville integrals are evaluated in Chapter 3. Numerical approximations based on polynomial interpolation, spectral methods, the fractional multistep method, and diffusive approximation are derived in detail. Some methods have convergence orders depending on the integral order α, while others have convergence orders for which α is irrelevant. Numerical examples are presented to directly display the effect of these numerical methods.

Viewing the Caputo derivative as a Riemann-Liouville integral of the integer-order derivative, we introduce a series of numerical approximations to the Caputo derivative in Chapter 4, based on the ideas introduced in Chapter 3. Replacing the given function by its polynomial interpolation, the L1, L2, and L2C methods, high-order methods based on polynomial interpolation, and spectral approximations can be readily obtained after direct calculating the Riemann-Liouville integral of integer-order derivatives of these interpolation functions. Diffusive approximation to the Caputo derivative can be derived analogously to the Riemann-Liouville integral. In view of the relationship between Caputo and Riemann-Liouville derivatives, fractional backward difference formulae for Caputo derivatives are also derived in Chapter 4. Apart from fractional backward difference formulae, which are of integer-order accuracy, numerical approximations introduced in Chapter 4 have error estimates depending on the derivative order α. This can be verified by numerical examples displayed in that chapter.

Numerical evaluations of Riemann-Liouville derivatives are introduced in Chapter 5. In view of numerical approximations to the Caputo derivative, the link between Caputo and Riemann-Liouville derivatives yields L1, L2, and L2C methods and spectral approximations to Riemann-Liouville derivatives. Other approaches approximating the Riemann-Liouville derivative in direct ways, including Grünwald-Letnikov type approximations, fractional backward difference formulae and their modifications, the fractional average central difference method, and the numerical method based on finite-part integrals, are also introduced, along with numerical examples.

Chapter 6 introduces numerical approximations to Riesz derivatives. According to the range of α, say $0 < \alpha < 1$ and $1 < \alpha < 2$, numerical methods are divided into two cases: one for the fractional convection operator and another for the fractional diffusion operator. Indirect methods follow from the observation that the Riesz derivative is a linear combination of left- and right-sided Riemann-Liouville derivatives. Direct methods are mainly derived from the asymmetric centered difference operator and its variants. The corresponding numerical examples are presented as well.

To emphasize the ubiquity of the integral definition of fractional Laplacian, the continuous time random walk process is considered in Chapter 7 to show its physical interpretations. Then the numerical methods for the fractional Laplacian in one space dimension are presented. Some relevant remarks are also included.

Overall, fundamental knowledge on fractional calculus along with comprehensive ideas introduced in this book provide the reader with better understanding of this subject, in terms of both pure theories and applications. The audience may benefit from the detailed derivation processes of the fruitful numerical approximations, since these derivation processes can give some hints on establishing some other novel numerical schemes. Accordingly, this book may indeed be a genuine guide to the central ideas of fractional calculus. In view of the fact that almost all the existing results on numerical approximations to fractional integrals and fractional derivatives are included in this book, it is appropriate to use it in educational classes as a detailed introduction to fractional calculus, as we move forward into a new era of the fractional world.

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