ON THE STABLE ESTIMATION OF RIEMANN-LIOUVILLE AND CAPUTO FRACTIONAL DERIVATIVES

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ABSTRACT

The computation of Riemann-Liouville and Caputo fractional derivatives in the presence of measured data is considered as an ill-posed problem and treated by mollification techniques. It is shown that, with the appropriate choice of the radius of mollification, the method is a regularizing algorithm, and the order of convergence is derived. Error estimates are included together with numerical examples of interest.

1. INTRODUCTION

Fractional derivatives and partial fractional derivatives have been applied recently to the numerical solution of problems in fluid and continuum mechanics [4], viscoelastic and viscoplastic flow [2] and anomalous diffusion (superdiffusion, non-Gaussian diffusion) [3], [5]. Numerous citations to several other applications of fractional derivatives to problems in physics, finance and hydrology can also be found in these articles.
The usual formulation of the fractional derivative, given in standard references such as [8], [10] and [9], is the Riemann Liouville definition.
The Riemann-Liouville fractional derivative of order $\alpha > 0$, of an integrable function g defined on the interval $[0, T]$, is given by the convolution integral

$$(D^{RL(\alpha)}g)(t) = \frac{1}{\Gamma(n-\alpha)}\frac{d^n}{dt^n}\int_0^t \frac{g(s)}{(t-s)^{\alpha+1-n}}\,ds,$$
$$0 \le t \le T, n-1 < \alpha < n, \, n \,\epsilon\, N,$$
$$(DRL^{(\alpha)}g)(t) = \frac{d^n g(t)}{dt^n},$$
$$0 \le t \le T, \, \alpha = n,$$

where $\Gamma(.)$ is the Gamma function and N indicates the set of natural numbers.
This definition leads to fractional differential equations which require the initial conditions to be expressed not in terms of the solution itself but rather in terms of its fractional derivatives, which are difficult to derive from a physical system. In applications it is often more convenient to use the formulation of the fractional derivative suggested by Caputo [1] which requires the same starting conditions as an ordinary differential equation of order n .

The Caputo fractional derivative of order $\alpha > 0$, of a differentiable function g defined on the interval $[0, T]$, is given by the convolution integral

$$(D^{(\alpha)}g)(t) = \frac{1}{\Gamma(n-\alpha)}\int_0^t \frac{g^{(n)}(s)}{(t-s)^{\alpha+1-n}}\,ds,$$
$$0 \le t \le T, n-1 < \alpha < n, n \epsilon N,$$
$$(DRL^{(\alpha)}g)(t) = \frac{d^n g(t)}{dt^n},$$
$$0 \le t \le T, \alpha = n.$$

One important difference between the Caputo fractional derivative and the Riemann-Liouville fractional derivative, besides the different requirements on the function g itself, is that the Caputo derivative of a constant is zero. For further details and relationships between these two types of fractional derivatives as well as a historical perspective on fractional derivatives in general, see [8].

Fractional differential operators are particular first kind Volterra integral equations (nonlocal operators) with weakly singular kernels and the above formulations are of little use in practice unless the data is known exactly.

The purpose of this paper is to present and analyze a stable method, based on mollification techniques, for the numerical computation of fractional derivatives when the data function $g^{(n-1)}$ is measured with noise.

The manuscript is organized as follows: in sections 2 the original ill-posed problem and the associated regularized (mollified) problem, respectively, are formulated. The numerical procedure, together with the stability and error analysis of the algorithm are investigated in section 3. Numerical examples are also provided in this section.

For basic properties and estimates associated with mollification in $\mathbf{R}^1$ the reader is referred to [7].

2. REGULARIZATION

Without loss of generality, we restrict our attention to functions defined on the interval $I = [0,1]$ and consider the case $n = 1$.

2.1 Caputo Fractional Derivatives

We would like to determine the Caputo fractional derivative of order α,

$$(D^{(\alpha)}g)(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{g'(s)}{(t-s)^{\alpha}}\, ds, \quad (2.1)$$
$$0 \le t \le 1,\ 0 < \alpha < 1,$$

from noisy data $g^{\varepsilon}(t)$, a perturbed version of the exact data function $g(t)$.

Equation (2.1) is a convolution integral equation that can also be expressed as

$$D^{(\alpha)}g = k * g',$$

where the kernel function k is given by

$$k(t) = \begin{cases} \dfrac{t^{-\alpha}}{\Gamma(1-\alpha)}, & t > 0, \\ 0, & t \le 0. \end{cases}$$

Instead of recovering $D^{(\alpha)}g$, in the presence of noise in the data, we look for a mollified solution $J_{\delta}(D^{(\alpha)}g^{\varepsilon})$ obtained from the previous equation by convolution with the Gaussian kernel ρ_{δ} (see [7]). Consequently, instead of equation (2.1), we have

$$J_{\delta}(D^{(\alpha)}g^{\varepsilon}) = D^{(\alpha)}g^{\varepsilon} * \rho_{\delta}$$
$$= k * (g^{\varepsilon} * \rho_{\delta})' = k * (J_{\delta}g^{\varepsilon})'.$$

That is, the mollified integral formula becomes, after suitable extension of the data function (see [7]),

$$J_{\delta}(D^{(\alpha)}g^{\varepsilon})(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{(J_{\delta}g^{\varepsilon})'(s)}{(t-s)^{\alpha}}\, ds. \quad (2.2)$$

The main properties of the method are given in the following theorem. The proof can be found in [7].

Theorem 2.1

If the functions g' and g^{ε} are uniformly Lipschitz on I and $\| g - g^{\varepsilon} \|_{\infty,I} \le \varepsilon$, then there exists a constant C, independent of δ, such that

$$\left\| J_{\delta}(D^{(\alpha)}g^{\varepsilon}) - D^{(\alpha)}g \right\|_{\infty, I}$$
$$\le C \frac{\delta + \dfrac{\varepsilon}{\delta}}{(1-\alpha)\Gamma(1-\alpha)}.$$

Stability is valid for each fixed $\delta > 0$ and the optimal rate of convergence is obtained by choosing $\delta = O(\sqrt{\varepsilon})$.

The mollified Caputo fractional derivative, reconstructed from noisy data, tends uniformly to the exact solution as $\epsilon \to 0,\ \delta = \delta(\epsilon) \to 0$.

This establishes the consistency, stability and convergence properties of the procedure.

2.1.1 Abstract Algorithm

The abstract algorithm based on the stable formula (2.2) is as follows:

1. Compute $J_{\delta}g^{\varepsilon}$ (this automatically provides $\delta = \delta(\varepsilon)$.)
2. Evaluate the derivative $(J_{\delta}g^{\varepsilon})'$ of the mollified data function $J_{\delta}g^{\varepsilon}$.

3. Use a quadrature formula to estimate $J_\delta(D^{(\alpha)}g)$ from equation (2.2).

2.2 Riemann-Liouville Fractional Derivatives

The evaluation of Riemann-Liouville fractional derivatives of order α,

$$(D^{RL(\alpha)}g)(t) = \frac{1}{\Gamma(1-\alpha)}\frac{d}{dt}\int_0^t \frac{g(s)}{(t-s)^\alpha}\,ds,$$
$$0 \le t \le 1,\ 0 < \alpha < 1, \qquad (2.3)$$

can be reduced to the treatment of Caputo's fractional derivatives under mild conditions on the function g. In practical situations it is possible to consider the discrete noisy data as the perturbed sample of an underlaying smooth (continuously differentiable) function. In this case, after integrating by parts, we get

$$(D^{RL(\alpha)}g)(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{g'(s)}{(t-s)^\alpha}\,ds + \frac{1}{\Gamma(1-\alpha)}\frac{g(0)}{t^\alpha},$$

or

$$(D^{RL(\alpha)}g)(t) = (D^{(\alpha)}g)(t) + \frac{1}{\Gamma(1-\alpha)}\frac{g(0)}{t^\alpha},$$

and we only need to estimate $(D^{(\alpha)}g)(t)$.

3. NUMERICAL PROCEDURE

To numerically approximate $J_\delta(D^{(\alpha)}g)$, a quadrature formula for the convolution equation (2.2) is needed. The objective is to introduce a simple quadrature and avoid any artificial smoothing in the process. To that effect, we consider a uniform partition K of the interval $I = [0,1]$, with elements $t_i = (i-1)\Delta t$, $i = 1,\dots,n$, $n\,\Delta t = 1$ and, after the noisy data function G^ε has been suitable extended and the radius of mollification automatically selected (see [7]), we define a piecewise constant interpolant of the corresponding mollified numerical derivative given by

$$\begin{aligned}(J_\delta l^\varepsilon)'(t) &= \mathbf{D}_+(J_\delta G^\varepsilon)(t_1)\varphi_1(t)\\ &+\sum_{i=2}^{j-1}\mathbf{D}_0(J_\delta G^\varepsilon)(t_i)\varphi_i(t)\\ &+\mathbf{D}_+(J_\delta G^\varepsilon)(t_j)\varphi_j(t),\\ &0 \le t \le t_j,\end{aligned}$$

where

$$\varphi_1(t) = \begin{cases}1 & \text{if } 0 \le t \le \Delta t/2\\ 0 & \text{otherwise}\end{cases},$$

$$\varphi_j(t) = \begin{cases}1 & \text{if } t_j - \Delta t/2 \le t \le t_j\\ 0 & \text{otherwise}\end{cases},$$

$$\varphi_i(t) = \begin{cases}1 & \text{if } t_i - \Delta t/2 \le t \le t_i + \Delta t/2\\ 0 & \text{otherwise}\end{cases},$$
$$i = 2,3,\dots,j-1,$$

and $\mathbf{D}_+$ and $\mathbf{D}_0$ represent the forward and centered finite difference approximations, respectively, to $(J_\delta G^\varepsilon)'$.

The discrete computed solution, denoted $(D^{(\alpha)}G^\varepsilon)_\delta$, is then obtained with the quadrature formula

$$(D^{(\alpha)}G^\varepsilon)_\delta(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{(J_\delta l^\varepsilon)'(s)}{(t-s)^\alpha}\,ds,$$

which, when restricted to the grid points, gives

$$\begin{aligned}(D^{(\alpha)}G^\varepsilon)_\delta(t_1) &= \mathbf{D}_+(J_\delta G^\varepsilon)(t_1)W_1,\\ (D^{(\alpha)}G^\varepsilon)_\delta(t_2) &= \mathbf{D}_+(J_\delta G^\varepsilon)(t_1)W_1\\ &\quad+\mathbf{D}_+(J_\delta G^\varepsilon)(t_2)W_2,\\ (D^{(\alpha)}G^\varepsilon)_\delta(t_j) &= \mathbf{D}_+(J_\delta G^\varepsilon)(t_1)W_1\\ &\quad+\sum_{i=2}^{j-1}\mathbf{D}_0(J_\delta G^\varepsilon)(t_i)W_{j-i+1}\\ &\quad+\mathbf{D}_+(J_\delta G^\varepsilon)(t_j)W_j,\\ &\quad j = 3,\dots,n.\end{aligned}$$

Here the quadrature weights $W_j(\alpha,\Delta t)$ are integrated exactly with values

$$W_1 = \frac{1}{\Gamma(1-\alpha)} \frac{1}{1-\alpha} (\frac{\Delta t}{2})^{1-\alpha},$$

$$W_i = \frac{1}{\Gamma(1-\alpha)} \frac{1}{1-\alpha} [((2i+1)\frac{\Delta t}{2})^{1-\alpha} - ((2i-1)\frac{\Delta t}{2})^{1-\alpha}],$$

$$i = 2, 3, \ldots, j-1,$$

and

$$W_j = \frac{1}{\Gamma(1-\alpha)} \frac{1}{1-\alpha} [j\Delta t - [(j-\frac{1}{2})\Delta t]^{1-\alpha}].$$

The error analysis is discussed next. The proof can be found in [6].

Theorem 3.1

If the functions g' *and* g^{ϵ} *are uniformly Lipschitz on* I *and* G and G^{ε}, *the discrete versions of* g *and* g^{ε} *respectively, satisfy* $\| G - G^{\epsilon} \|_{\infty,K} \leq \epsilon$, *then:*

$$\left\| J_{\delta}(D^{(\alpha)} g^{\varepsilon}) - (D^{(\alpha)} G^{\varepsilon})_{\delta} \right\|_{\infty,K} \leq \frac{C}{\Gamma(1-\alpha)} \times \frac{\Delta t}{1-\alpha}.$$

Corollary 3.2

Under the hypothesis of Theorems 2.1 and 3.1,

$$\left\| (D^{(\alpha)} G^{\varepsilon})_{\delta} - D^{(\alpha)} g \right\|_{\infty,K} \leq \frac{C}{\Gamma(1-\alpha)} \times \frac{\delta + \frac{\epsilon}{\delta} + \Delta t}{1-\alpha}.$$

The error estimate for the discrete case is obtained by adding the global truncation error to the error estimate of the nondiscrete case.

3.1 Numerical Results

In this subsection we discuss some numerical tests performed with the algorithm introduced in the previous sections.

The discretization parameters are as follows: the number of time divisions is n, $\Delta t = 1/(n-1)$ and $t_i = (i-1)\Delta t$, $i = 1, 2, \ldots, n$. The use of the average perturbation value ε is only necessary for the purpose of generating the noisy data for the simulations. The filtering procedure automatically adapts the regularization parameter to the quality of the data [7].

Discretized measured approximations of the data are simulated by adding random errors to the exact data functions. Specifically, for an exact data function g, its discrete noisy version is

$$G^{\varepsilon}(t_i) = g(t_i) + \varepsilon_i, \quad |\varepsilon_i| \leq \varepsilon, \; i = 1, 2, \ldots, n,$$

where the $(\varepsilon_i)'s$ are Gaussian random variables with variance $\sigma^2 = \varepsilon^2$.

In order to test the stability and accuracy of the algorithm, we consider two examples and a selection of average noise perturbations. The fractional derivative errors are measured by the relative weighted l^2- norms defined by

$$\frac{\left[\frac{1}{n} \sum_{n=1}^{n} \left| (D^{(\alpha)} G^{\varepsilon})_{\delta}(t_i) - D^{(\alpha)} g(t_i) \right|^2 \right]^{1/2}}{\left[\frac{1}{n} \sum_{n=1}^{n} \left| D^{(\alpha)} g(t_i) \right|^2 \right]^{1/2}}.$$

In the examples that follow, we observe that $\frac{1}{\sqrt{\pi}} D^{(0.5)} g$ is the Abel's transform of g and also that $D^{(0.99)} g$ can be interpreted as an approximation to the ordinary derivative g'.

Example 1

The exact data in this example is provided by the identity function $g(t) = t, \; 0 \leq t \leq 1$. The exact Caputo fractional derivatives are given by $D^{(\alpha)} g(t) = \frac{1}{\Gamma(1-\alpha)} \frac{t^{1-\alpha}}{1-\alpha}$, $0 < \alpha < 1$, $0 \leq t \leq 1$.

The relative errors in the approximation of the fractional derivatives as functions of the amount of noise in the data are shown in Table 3.1. A graphical illustration of the exact and computed fractional derivatives appears in Figure 3.1.

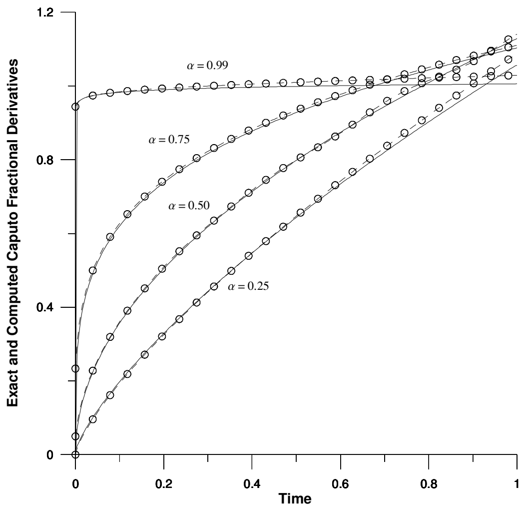

Fig. 3.1. Example 1. Exact and computed (- o -) fractional derivative functions with parameters $\Delta t = 1/256$ and $\varepsilon = 0.1$.

Relative l^2 – Norm Fractional Derivative Errors				
$\varepsilon \setminus \alpha$	0.25	0.50	0.75	0.99
0.00	0.0023	0.0041	0.0148	0.0591
0.05	0.0016	0.0066	0.0159	0.0599
0.10	0.0017	0.0063	0.0162	0.0604

Table 3.1. Example 1. Fractional derivative errors as functions of ε for $\Delta t = 1/256$.

Example 2

The exact data function and Caputo fractional derivatives are, respectively, $g(t) = t^2$ and $\frac{\Gamma(3)}{\Gamma(3-\alpha)} t^{2-\alpha}$, $0 < \alpha < 1$, $0 \le t \le 1$.

The relative errors in the approximation of the fractional derivatives as functions of the amount of noise in the data are shown in Table 3.2. A graphical illustration of the exact and computed fractional derivatives is provided in Figure 3.2.

In all cases, stability with respect to perturbations in the data has been restored and the physical quality of the numerical reconstructions is quite acceptable even in the presence of relatively large amounts of noise in the data. As α increases, the problems become more ill-posed, and for each noise level the relative errors increase accordingly, as expected.

Relative l^2 – Norm Fractional Derivative Errors				
$\varepsilon \setminus \alpha$	0.25	0.50	0.75	0.99
0.00	0.0043	0.0060	0.0083	0.0095
0.05	0.0033	0.0089	0.0105	0.0148
0.10	0.0075	0.0014	0.0225	0.0668

Table 3.2. Example 2. Fractional derivative errors as functions of ε for $\Delta t = 1/256$.

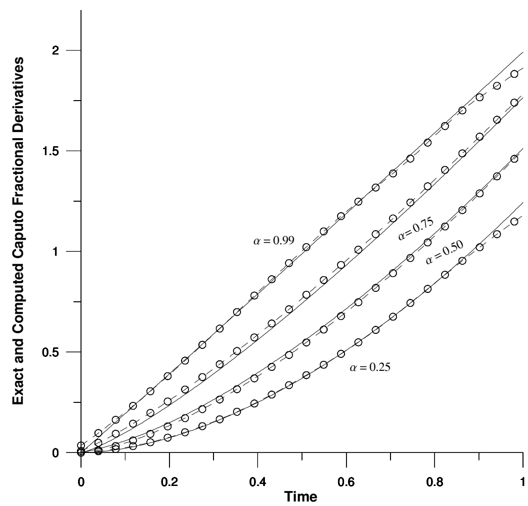

Fig. 3.2. Example 2. Exact and computed (- o -) fractional derivative functions with parameters $\Delta t = 1/256$ and $\varepsilon = 0.1$.

Acknowledgment

This work was partially supported by a C. P. Taft fellowship.

4. REFERENCES

1. M. Caputo, *Elastica e Dissipazione*, Zanichelli, Bologna, (1969)

2. K. Diethelm and A. D. Freed, On the solution of nonlinear fractional order differential equations used in the modelling of viscoplasticity, *Scientific Computing in Chemical Engineering II*: *Computational Fluid Dynamics, Reaction Engineering and Molecular Properties*, Springer Verlag, Heidelberg, 217-224, (1999)

3. F. Liu, V. Anh and I. Turner, Numerical solution of the space fractional Fokker-Planck

equation, *JCAM*, 166 209-219, (2004)

4. F. Mainardi, *Fractals and Fractional Calculus Continuum Mechanics*, Springer Verlag, 291-348, (1997)

5. M. M. Meerschaert and C. Tadjeran, Finite difference approximations for fractional advection-dispersion flow equations, *JCAM*, 172, 65-77, (2004)

6. D. A. Murio, On the Stable Computation of Caputo Fractional Derivatives, *Computers Math. Applic.*, to appear in (2006)

7. D. A. Murio, Mollification and Space Marching, Chapter 4 in *Inverse Engineering Handbook*, K. Woodbury Ed., CRC Press, Boca Raton, Florida, (2002)

8. I. Podlubny, *Fractional Differential Equations*, Academic Press, (1999)

9. K. B. Oldman and J. Spanier, *The Fractional Calculus*, Academic Press, (1974)

10. S. G. Samko, A. A. Kilbas and O. I. Marichev, *Fractional Integrals and Derivatives*, Gordan and Breach Sciences Publishers, (1993)