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RESEARCH PAPER

FORMAL CONSISTENCY VERSUS ACTUAL CONVERGENCE RATES OF DIFFERENCE SCHEMES FOR FRACTIONAL-DERIVATIVE BOUNDARY VALUE PROBLEMS

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Abstract

Finite difference methods for approximating fractional derivatives are often analyzed by determining their order of consistency when applied to smooth functions, but the relationship between this measure and their actual numerical performance is unclear. Thus in this paper several well-known difference schemes are tested numerically on simple Riemann-Liouville and Caputo boundary value problems posed on the interval $[0,1]$ to determine their orders of convergence (in the discrete maximum norm) in two unexceptional cases: (i) when the solution of the boundary-value problem is a polynomial (ii) when the data of the boundary value problem is smooth. In many cases these tests reveal gaps between a method's theoretical order of consistency and its actual order of convergence. In particular, numerical results show that the popular shifted Grünwald-Letnikov scheme fails to converge for a Riemann-Liouville example with a polynomial solution $p(x)$, and a rigorous proof is given that this scheme (and some other schemes) cannot yield a convergent solution when $p(0) \neq 0$.

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1. **Introduction**

In this paper we are concerned with two-point boundary value problems whose highest-order derivative is a fractional derivative of order δ, with $1 < \delta < 2$. That is, we consider the differential equation

$$Lu(x) := D^\delta u(x) + b(x)u'(x) + c(x)u(x) = f(x) \quad \text{for} \quad x \in (0,1), \tag{1.1}$$

together with some appropriate boundary conditions at $x = 0$ and $x = 1$ that we will specify later. Here D^δ is a fractional derivative of either Riemann-Liouville or Caputo type; these terms are defined below.

For $n = 1, 2, \ldots$, denote by $A^n[0,1]$ the set of functions $g \in C^{n-1}[0,1]$ with $g^{(n-1)}$ absolutely continuous on [0,1], i.e., $g^{(n)}$ exists almost everywhere in [0,1] and

$$g^{(n-1)}(x) = g^{(n-1)}(0) + \int_{t=0}^{x} g^{(n)}(t)\,dt \quad \text{for} \quad 0 \le x \le 1.$$

Clearly, $C^n[0,1] \subset A^n[0,1]$.

For $r \in \mathbb{R}$ with $r > 0$, and all g in the Lebesgue space $L_1[0,1]$, define the *Riemann-Liouville fractional integral operator* of order r by

$$(J^r g)(x) = \left[\frac{1}{\Gamma(r)} \int_{t=0}^{x} (x-t)^{r-1} g(t)\,dt\right] \quad \text{for} \quad 0 \le x \le 1. \tag{1.2}$$

Recall that $1 < \delta < 2$. Assume that $g \in A^2[0,1]$. Then the *Riemann-Liouville fractional derivative* D^δ_{RL} is defined by

$$D^\delta_{RL} g(x) = \left(\frac{d}{dx}\right)^2 (J^{2-\delta} g)(x) \quad \text{for} \quad 0 < x \le 1, \tag{1.3}$$

and the *Caputo fractional derivative* D^δ_C is defined [1, Definition 3.2] in terms of D^δ_{RL} by

$$D^\delta_C g = D^\delta_{RL}[g - T_1[g;0]], \tag{1.4}$$

where $T_1[g;0]$ denotes the Taylor polynomial of degree 1 of the function g expanded around $x = 0$. By [1, Theorem 3.1] one also has the equivalent formulation

$$D^\delta_C g(x) = \frac{1}{\Gamma(2-\delta)} \int_{t=0}^{x} (x-t)^{1-\delta} g''(t)\,dt \quad \text{for} \quad 0 < x \le 1. \tag{1.5}$$

In recent decades, a wide range of physical processes – in, e.g., physics, finance, biology and chemistry – have been modelled using fractional differential equations, and consequently the investigation of solutions of these equations has received considerable attention (see for example [6] and its references). Many papers have considered finite difference methods for (1.1) and for its time-dependent analogue where $u = u(x,t)$ and a time derivative of u (of integer or fractional order) also appears in the differential equation. In almost all of this published work, the accuracy of the numerical method has been judged by performing Taylor expansions (e.g., [11, 12, 14]) or Fourier analysis (e.g., [7, 16, 17]) to estimate the truncation error, while assuming that the derivatives of u that are needed in this analysis are bounded. This provides useful information about the properties of these methods, but it leaves open the question of how accurate these methods are when they are applied to problems whose solutions u are less well behaved—and as we shall see shortly, this lack of smoothness in u is common when the right-hand side f is smooth. Our mission in the present paper is to investigate numerically and theoretically how well various numerical methods in the research literature perform when applied to solutions of (1.1) that are of two types:

(i) well-behaved, i.e., with bounded derivatives;
(ii) less well-behaved, i.e., typical of solutions of (1.1) when the function f is smooth, which is a reasonable assumption in practice.

Thus our results will extend the results of the earlier papers by showing how accurate their methods are when applied to more difficult (but realistic) problems.

Our paper is structured as follows. In Section 2 we describe the two examples that will be used to test the orders of convergence (in the discrete maximum norm) of the finite difference schemes, and introduce some terminology common to all these methods. Section 3 presents numerical results when the L2 scheme [8] and the spline-based scheme [12] are used to approximate an example with a Caputo fractional derivative. The Riemann-Liouville fractional derivative is investigated numerically in Section 4, where we consider the classical L2 scheme [8], some schemes based on the shifted and weighted Grünwald-Letnikov formula [7, 16, 17], and a spline-based scheme of [14]. Furthermore, Section 4.5 provides a rigorous proof that when the solution of the boundary value problem is a polynomial $p(x)$, the well-known shifted Grünwald-Letnikov scheme [7] fails to converge if $p(0) \neq 0$. The schemes of [14, 16] are similarly deficient.

2. **Our test problems**

Throughout the paper we shall use as test problems the following two examples, which correspond to the two types of problem described in the previous section. In both we simplify (1.1) by taking $b = c \equiv 0$ in order to focus attention on the effects of different discretizations of the fractional derivative term in (1.1). Each example comprises a test problem for D^{δ}_{RL} and a test problem for D^{δ}_{C}.

Example 2.1. (Smooth solution u, nonsmooth f) Consider the differential equation

$$D^\delta u(x) = f(x) \quad \text{for} \quad x \in (0,1), \tag{2.1}$$

with Dirichlet boundary conditions $u(0) = 1,\ u(1) = -1$, where the function f is chosen such that $u(x) = 1+3x-7x^2+4x^3-2x^4$ is the exact solution of this boundary value problem. Here we remind the reader that D^δ can be the Riemann-Liouville derivative D^δ_{RL} or the Caputo derivative D^δ_C.

When $D^\delta = D^\delta_{RL}$, then by [1, Example 2.4] we have

$$f(x) = \frac{x^{-\delta}}{\Gamma(1-\delta)} + \frac{3x^{1-\delta}}{\Gamma(2-\delta)} - \frac{14x^{2-\delta}}{\Gamma(3-\delta)} + \frac{24x^{3-\delta}}{\Gamma(4-\delta)} - \frac{48x^{4-\delta}}{\Gamma(5-\delta)}\,.$$

While $u \in C^\infty[0,1]$, one has $f \in C^\infty(0,1]$ but $f \notin C[0,1]$.

When $D^\delta = D^\delta_C$, then by [1, Appendix B] we have

$$f(x) = -\frac{14x^{2-\delta}}{\Gamma(3-\delta)} + \frac{24x^{3-\delta}}{\Gamma(4-\delta)} - \frac{48x^{4-\delta}}{\Gamma(5-\delta)}\,.$$

Now $f \in C^\infty(0,1] \cap C[0,1]$ but $f \notin C^1[0,1]$.

Example 2.2. (Smooth f, nonsmooth solution u) Consider the differential equation

$$D^\delta u(x) = 1 \quad \text{for} \quad x \in (0,1), \tag{2.2}$$

with Dirichlet boundary conditions $u(0) = 0,\ u(1) = 2$. Thus we have chosen $f(x) \equiv 1$.

When $D^\delta = D^\delta_{RL}$, then from [1, p.54] it follows that

$$u(x) = \frac{x^\delta}{\Gamma(1+\delta)} + \left[2 - \frac{1}{\Gamma(1+\delta)}\right] x^{\delta-1}.$$

While $f \in C^\infty[0,1]$, one has $u \in C[0,1] \cap C^\infty(0,1]$ but $u \notin C^1[0,1]$.

Note here that the general solution of the differential equation $D^\delta_{RL} u = 1$ includes a term $kx^{\delta-2}$ (for some constant k), which implies that the only possible value for the Dirichlet condition at $x = 0$ is the homogeneous choice $u(0) = 0$ to force $k = 0$ (otherwise $u(0)$ would not be defined). Some authors deal with this troublesome term in a different way, by specifying the value of $\lim_{x\to 0} x^{2-\delta} u(x)$, but the physical interpretation of this type of boundary condition is contentious so we do not consider this possibility here.

When $D^\delta = D^\delta_C$, then from [1, p.55] it follows that

$$u(x) = \frac{x^\delta}{\Gamma(1+\delta)} + \left[2 - \frac{1}{\Gamma(1+\delta)}\right] x.$$

Thus $u \in C^1[0,1] \cap C^\infty(0,1]$ but $u \notin C^2[0,1]$.

REMARK 2.1. (Other boundary conditions) The papers [3, 4, 15] consider the problem (1.1) with $D^\delta = D_C^\delta$ but with a Robin boundary condition at $x = 0$. This boundary condition is needed to ensure that the boundary value problem satisfies a maximum principle – a useful property that facilitates the analysis in these papers. We do not consider this type of boundary condition here because its discretization would introduce a further element of variability into our investigations, thereby weakening our focus on the behaviour of different discretizations of the fractional derivative D_C^δ.

The solution v of the problem considered in the three papers mentioned in Remark 2.1 is analyzed thoroughly in [15] and it is shown that $v \in C^1[0,1] \cap C^\infty(0,1]$ but in general $v \notin C^2[0,1]$. Thus the lack of smoothness in the solution to $D_C^\delta u = 1$ that we observed in Example 2.2 carries over to the general case of (1.1).

2.1. **Formal order of consistency, mesh, tables.** In the sections that follow, each difference scheme has a "formal order of consistency". By this we mean the order of consistency that the scheme attains when its truncation error is estimated using Taylor expansions under the assumption that the derivatives in these expansions are bounded by some fixed constant on all of $[0,1]$, as is frequently done in the literature.

We use the uniform mesh $x_j = jh$ for $j = 0, 1, \ldots, N$ where N is a positive integer and $h := 1/N$. In all our difference schemes the right-hand side f of the differential equation is approximated at x_j by $f(x_j)$.

Write the computed solution of each scheme as $\{u_j : \ j = 0, \ldots, N\}$. Each table of numerical results in the following sections displays the maximum nodal error

$$e_N^\delta := \max_{0 \le j \le N} |u(x_j) - u_j|,$$

of a particular scheme applied to an example from Section 2 for a range of values of N and δ. The orders of convergence p_N^δ are then computed in the standard way:

$$p_N^\delta := \log_2 \left(\frac{e_N^\delta}{e_{2N}^\delta} \right).$$

We shall see that in some cases the rate of convergence attained by a scheme depends on the value of δ.

3. Caputo derivative: numerical results

This section examines the numerical behaviour of two well-known difference schemes that are used to solve Examples 2.1 and 2.2 with $D^\delta = D_C^\delta$.

3.1. **The L2 scheme.** This scheme is described in [5] and [13], and it was also used in [15]. For a proof that it is formally first-order consistent, see [11].

The L2 scheme approximates the Caputo fractional derivative by

$$D_C^\delta u(x_j) \approx \frac{1}{h^\delta\,\Gamma(3-\delta)} \sum_{k=0}^{j-1} d_{j-k}\left(u_{k+2} - 2u_{k+1} + u_k\right), \tag{3.1}$$

where we set

$$d_r = r_+^{2-\delta} - (r-1)_+^{2-\delta} \quad \text{for all integers } r \tag{3.2}$$

and

$$s_+ = \begin{cases} s & \text{if } s \geq 0, \\ 0 & \text{if } s < 0. \end{cases}$$

Note that $d_r = 0$ for $r \leq 0$. The numerical results in Tables 1 and 2 show that when it is applied to Examples 2.1 and 2.2 with $D^\delta = D_C^\delta$, one obtains first-order convergence in both cases, i.e., the order of convergence agrees with the formal order of consistency.

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	6.45(-3)	3.12(-3)	1.53(-3)	7.60(-4)	3.78(-4)	1.89(-4)
	1.045	1.025	1.014	1.008	1.004	
$\delta = 1.3$	6.68(-3)	3.22(-3)	1.57(-3)	7.73(-4)	3.82(-4)	1.90(-4)
	1.050	1.036	1.024	1.015	1.010	
$\delta = 1.5$	6.78(-3)	3.31(-3)	1.61(-3)	7.92(-4)	3.90(-4)	1.93(-4)
	1.035	1.035	1.028	1.021	1.015	
$\delta = 1.7$	6.10(-3)	3.11(-3)	1.56(-3)	7.78(-4)	3.86(-4)	1.92(-4)
	0.972	0.998	1.006	1.008	1.007	
$\delta = 1.9$	3.08(-3)	1.74(-3)	9.35(-4)	4.91(-4)	2.55(-4)	1.32(-4)
	0.824	0.895	0.929	0.945	0.955	

TABLE 1. Example 2.1 with $D^\delta = D_C^\delta$: L2 scheme

3.2. **Spline-based scheme** [12]**.** This scheme appears in [13]; its source is [12], where it is shown in [12, Theorem 1] to be formally second-order consistent if $u \in C^4[0,1]$. Now the Caputo fractional derivative is approximated by

$$\begin{aligned} D_C^\delta u(x_j) \approx \frac{1}{h^\delta\,\Gamma(4-\delta)} \Big\{ & a_{j0}(2u_0 - 5u_1 + 4u_2 - u_3) \\ & + \sum_{k=1}^{j} a_{jk}\left(u_{k+1} - 2u_k + u_{k-1}\right) \Big\}, \end{aligned} \tag{3.3}$$

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	2.23(-2) 0.981	1.13(-2) 0.990	5.68(-3) 0.995	2.85(-3) 0.998	1.43(-3) 0.999	7.15(-4)
$\delta = 1.3$	1.36(-2) 0.959	7.02(-3) 0.978	3.56(-3) 0.988	1.80(-3) 0.993	9.03(-4) 0.996	4.53(-4)
$\delta = 1.5$	7.56(-3) 0.922	3.99(-3) 0.951	2.06(-3) 0.969	1.05(-3) 0.980	5.35(-4) 0.986	2.70(-4)
$\delta = 1.7$	3.04(-3) 0.858	1.67(-3) 0.901	8.97(-4) 0.928	4.71(-4) 0.947	2.45(-4) 0.959	1.26(-4)
$\delta = 1.9$	3.74(-4) 0.752	2.22(-4) 0.812	1.27(-4) 0.852	7.01(-5) 0.878	3.82(-5) 0.898	2.05(-5)

TABLE 2. Example 2.2 with $D^\delta = D^\delta_C$: L2 scheme

where

$$a_{jk} = \begin{cases} (j-1)^{3-\delta} - j^{2-\delta}(j-3+\delta) & \text{if } k = 0, \\ (j-k+1)^{3-\delta} - 2(j-k)^{3-\delta} + (j-k-1)^{3-\delta} & \text{if } 1 \le k \le j-1, \\ 1 & \text{if } k = j. \end{cases}$$

In Example 2.1 with $D^\delta = D^\delta_C$, this scheme attains second-order convergence, as exhibited in Table 3. But in Example 2.2 with $D^\delta = D^\delta_C$, the scheme is only first-order convergent – see Table 4. Thus our numerical results seem to indicate that the order of convergence of the scheme (3.3) is reduced below the order of consistency if the solution of the boundary value problem is nonsmooth.

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	9.75(-4) 1.998	2.44(-4) 1.999	6.10(-5) 2.000	1.53(-5) 2.000	3.81(-6) 2.000	9.54(-7)
$\delta = 1.3$	9.70(-4) 1.994	2.43(-4) 1.998	6.10(-5) 1.999	1.52(-5) 2.000	3.81(-6) 2.000	9.53(-7)
$\delta = 1.5$	9.50(-4) 1.984	2.40(-4) 1.992	6.04(-5) 1.995	1.52(-5) 1.997	3.80(-6) 1.998	9.51(-7)
$\delta = 1.7$	8.84(-4) 1.961	2.27(-4) 1.976	5.77(-5) 1.983	1.46(-5) 1.987	3.68(-6) 1.990	9.27(-7)
$\delta = 1.9$	6.87(-4) 1.945	1.79(-4) 1.958	4.60(-5) 1.966	1.18(-5) 1.970	3.00(-6) 1.974	7.65(-7)

TABLE 3. Example 2.1 with $D^\delta = D^\delta_C$: spline-based scheme [12]

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	5.36(-3)	2.54(-3)	1.20(-3)	5.62(-4)	2.82(-4)	1.48(-4)
	1.077	1.087	1.089	0.997	0.928	
$\delta = 1.3$	2.61(-3)	1.44(-3)	7.83(-4)	4.18(-4)	2.20(-4)	1.15(-4)
	0.859	0.881	0.905	0.925	0.941	
$\delta = 1.5$	1.40(-3)	7.78(-4)	4.21(-4)	2.22(-4)	1.16(-4)	5.95(-5)
	0.845	0.888	0.920	0.943	0.959	
$\delta = 1.7$	4.79(-4)	2.70(-4)	1.46(-4)	7.71(-5)	3.99(-5)	2.04(-5)
	0.827	0.885	0.924	0.951	0.968	
$\delta = 1.9$	3.87(-5)	2.47(-5)	1.42(-5)	7.69(-6)	4.03(-6)	2.07(-6)
	0.646	0.800	0.883	0.931	0.960	

TABLE 4. Example 2.2 with $D^\delta = D^\delta_C$: spline-based scheme [12]

4. Riemann-Liouville derivative: numerical results

Now we move on to examine the numerical behaviour of several well-known difference schemes that are used to solve Examples 2.1 and 2.2 with $D^\delta = D^\delta_{RL}$. These experiments will show a more widespread discrepancy between the formal consistency order and the order of convergence than was the case for the Caputo boundary value problems of Section 3.

In particular, our experiments will show that the solution of the well-known shifted Grünwald-Letnikov scheme does *not* converge to the solution of Example 2.1 as the mesh diameter goes to zero; later, in Section 4.5, we give a rigorous proof that this scheme cannot attain any positive order of convergence for this problem.

4.1. **The L2 scheme.** The L2 scheme [8, p.140] discretization of $D^\delta_{RL} u(x) = f$ is

$$\frac{1}{h^\delta\,\Gamma(3-\delta)}\sum_{k=0}^{j-1} d_{j-k}\,(u_{k+2}-2u_{k+1}+u_k) + \frac{u_0(x_j-x_0)^{-\delta}}{\Gamma(1-\delta)} + \frac{(u_1-u_0)(x_j-x_0)^{1-\delta}}{(x_1-x_0)\Gamma(2-\delta)} = f(x_j) \quad \text{for} \quad j = 1,2,\dots,N-1, \tag{4.1}$$

where the coefficients d_j are defined in (3.2).

This scheme is motivated by the following well-known relationship between the Riemann-Liouville and Caputo derivatives [1, Lemma 3.4]:

$$D^\delta_{RL} u(x) = \frac{u(0)x^{-\delta}}{\Gamma(1-\delta)} + \frac{u'(0)x^{1-\delta}}{\Gamma(2-\delta)} + D^\delta_C u(x). \tag{4.2}$$

Now one applies the L2 scheme of Section 3.1 to discretize the Caputo derivative and a simple forward difference to discretize $u'(0)$. As both of these discretizations are formally first-order consistent, the L2 scheme (4.1) is also formally first-order consistent.

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	1.15(-1)	5.88(-2)	2.95(-2)	1.45(-2)	7.37(-3)	3.67(-3)
	0.976	0.993	1.000	1.004	1.006	
$\delta = 1.3$	6.84(-2)	3.42(-2)	1.69(-2)	8.31(-3)	4.09(-3)	2.01(-3)
	1.001	1.017	1.023	1.024	1.022	
$\delta = 1.5$	3.72(-2)	1.84(-2)	9.01(-3)	4.42(-3)	2.18(-3)	1.08(-3)
	1.021	1.028	1.026	1.021	1.016	
$\delta = 1.7$	1.76(-2)	8.72(-3)	4.36(-3)	2.19(-3)	1.10(-3)	5.54(-4)
	1.012	1.001	0.994	0.991	0.990	
$\delta = 1.9$	5.21(-3)	2.59(-3)	1.32(-3)	6.82(-4)	3.54(-4)	1.84(-4)
	1.010	0.970	0.953	0.947	0.947	

TABLE 5. Example 2.1 with $D^\delta = D^\delta_{RL}$: scheme L2

Tables 5 and 6 display the numerical results when the L2 scheme is used to solve Examples 2.1 and 2.2, respectively. These results show that the L2 scheme is first-order convergent if the solution is smooth but a reduction in the order of convergence is observed if the solution is not smooth—in fact when δ is near 1 in Table 6, the scheme fails to converge. Thus the behaviour of the L2 scheme for Riemann-Liouville derivatives is not the same as its behaviour for Caputo derivatives.

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	7.10(-2)	8.51(-2)	9.72(-2)	1.08(-1)	1.16(-1)	1.23(-1)
	-0.261	-0.192	-0.149	-0.112	-0.082	
$\delta = 1.3$	6.88(-2)	7.29(-2)	7.24(-2)	6.88(-2)	6.32(-2)	5.67(-2)
	-0.084	0.009	0.075	0.122	0.157	
$\delta = 1.5$	3.20(-2)	3.05(-2)	2.68(-2)	2.23(-2)	1.79(-2)	1.40(-2)
	0.069	0.185	0.264	0.319	0.360	
$\delta = 1.7$	8.91(-3)	8.14(-3)	6.70(-3)	5.14(-3)	3.75(-3)	2.65(-3)
	0.130	0.282	0.383	0.453	0.504	
$\delta = 1.9$	1.83(-3)	1.01(-3)	5.48(-4)	3.43(-4)	2.51(-4)	1.73(-4)
	0.857	0.882	0.673	0.453	0.535	

TABLE 6. Example 2.2 with $D^\delta = D^\delta_{RL}$: scheme L2

4.2. **Shifted Grünwald-Letnikov scheme.** This scheme is a variant of an earlier scheme proposed independently by Grünwald and Letnikov: see [8, p.136] and [10]. Schemes based on the Grünwald and Letnikov formula with a shifting parameter were also considered, for example, in [2] and [8]. The variant that we discuss is the best known; its popularity grew after it was recommended in [7].

The shifted Grünwald-Letnikov approximation of $D^\delta_{RL}u(x) = f$ is

$$D^{\delta,N}_{GL,S}u_j := \frac{1}{h^\delta}\sum_{k=0}^{j+1} w_k^{(\delta)} u_{j-k+1} = f(x_j) \quad \text{for} \quad j = 1, 2, \ldots, N-1, \tag{4.3}$$

where

$$w_k^{(\delta)} := (-1)^k \binom{\delta}{k} = \frac{\Gamma(k-\delta)}{\Gamma(-\delta)\Gamma(k+1)}.$$

To compute the coefficients $w_k^{(\delta)}$ one can use the recurrence relation

$$w_0^{(\delta)} = 1, \quad w_k^{(\delta)} = \left(1 - \frac{\delta+1}{k}\right) w_{k-1}^{(\delta)} \text{ for } k = 1, 2, \ldots, j+1. \tag{4.4}$$

In [7, Theorem 2.7] it is proved that the approximation (4.3) is formally first-order consistent provided that the extension of the domain of definition of u to $\{x : x < 0\}$ by the function zero yields a function that lies in $C^{\delta+1}(-\infty, 1]$, so that [7, Theorem 2.4] can be invoked. A necessary condition for this extension requirement is that $0 = u(0) = u'(0) = u''(0)$, which is not satisfied by either of our examples.

An alternative argument in [13, Proposition 4], based on [10, Section 7.4], shows that for the polynomial solution of Example 2.1, the shifted Grünwald-Letnikov approximation is formally first-order consistent.

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	7.71(-2) 0.980	3.91(-2) -0.743	6.55(-2) -0.259	7.84(-2) -0.111	8.46(-2) -0.051	8.76(-2)
$\delta = 1.3$	1.53(-1) -0.251	1.82(-1) -0.107	1.96(-1) -0.048	2.03(-1) -0.022	2.06(-1) -0.010	2.07(-1)
$\delta = 1.5$	2.06(-1) -0.107	2.22(-1) -0.050	2.30(-1) -0.023	2.33(-1) -0.011	2.35(-1) -0.005	2.36(-1)
$\delta = 1.7$	1.66(-1) -0.063	1.73(-1) -0.031	1.77(-1) -0.015	1.79(-1) -0.007	1.80(-1) -0.004	1.80(-1)
$\delta = 1.9$	6.84(-2) -0.090	7.28(-2) -0.046	7.51(-2) -0.028	7.66(-2) -0.014	7.74(-2) -0.007	7.78(-2)

TABLE 7. Example 2.1 with $D^\delta = D^\delta_{RL}$: shifted G-L scheme

The numerical results in Table 7 for Example 2.1 seem to indicate that for all values of δ, the shifted Grünwald-Letnikov scheme fails to converge as $N \to \infty$. This is indeed what happens – we shall prove rigorously in Section 4.5 that for polynomial solutions (such as Example 2.1) this scheme fails to converge when $u(0) \neq 0$.

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	3.50(-2) 0.082	3.31(-2) 0.091	3.11(-2) 0.096	2.91(-2) 0.098	2.72(-2) 0.099	2.54(-2)
$\delta = 1.3$	4.03(-2) 0.280	3.32(-2) 0.290	2.71(-2) 0.295	2.21(-2) 0.298	1.80(-2) 0.299	1.46(-2)
$\delta = 1.5$	2.43(-2) 0.478	1.75(-2) 0.489	1.24(-2) 0.495	8.84(-3) 0.497	6.26(-3) 0.499	4.43(-3)
$\delta = 1.7$	1.05(-2) 0.675	6.61(-3) 0.688	4.10(-3) 0.694	2.54(-3) 0.697	1.56(-3) 0.698	9.64(-4)
$\delta = 1.9$	2.36(-3) 0.873	1.29(-3) 0.880	7.02(-4) 0.888	3.79(-4) 0.894	2.04(-4) 0.897	1.10(-4)

TABLE 8. Example 2.2 with $D^\delta = D^\delta_{RL}$: shifted G-L scheme

The solution of Example 2.2 is less smooth than the solution of Example 2.1 but it does have the helpful property $u(0) = 0$. Numerical results for this example are displayed in Table 8 and they indicate that the method is $O(h^{\delta-1})$ accurate. That is, the order of convergence of the method is reduced and the degree of reduction depends on the order of the Riemann-Liouville fractional derivative.

4.3. **Weighted and shifted Grünwald-Letnikov scheme** [16]**.** The scheme was introduced in [16] and is reproduced in [17]. The approximation used is

$$D^\delta_{RL} u(x_j) \approx \frac{1}{h^\delta} \sum_{k=0}^{j+p} w_k^{(\delta)} \left[\frac{\delta - 2q}{2(p-q)} u_{j-(k-p)} + \frac{2p-\delta}{2(p-q)} u_{j-(k-q)} \right],$$

where the coefficients $w_k^{(\delta)}$ are defined in (4.4) and p, q are integers with $p > q$. In [16] the authors recommend $(p, q) = (1, 0)$ and $(p, q) = (1, -1)$.

In [16, Remark 2.6] it is asserted that both these schemes are formally second-order consistent under the assumption $u(0) = 0$; the function u is extended by zero on $(-\infty, 0)$ and [16, Theorem 2.4] is then invoked – but the extension is not smooth at $x = 0$ so the hypotheses of [16, Theorem 2.4] are not satisfied.

We shall present numerical results only for $(p, q) = (1, 0)$ as the results for $(p, q) = (1, -1)$ are broadly similar. Tables 9 and 10 are for Examples 2.1

and 2.2 respectively, with $D^\delta = D^\delta_{RL}$. In Example 2.1 the scheme fails to converge for all values of δ, while for Example 2.2 the scheme is $O(h^{\delta-1})$ convergent. These are the same orders of convergence that we observed for the shifted Grünwald-Letnikov scheme (4.3).

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	8.37(-2) 0.014	8.29(-2) 0.003	8.27(-2) 0.001	8.27(-2) -0.000	8.27(-2) -0.000	8.27(-2)
$\delta = 1.3$	1.62(-1) 0.016	1.60(-1) 0.005	1.60(-1) 0.002	1.60(-1) 0.001	1.60(-1) 0.000	1.60(-1)
$\delta = 1.5$	1.53(-1) 0.024	1.51(-1) 0.009	1.50(-1) 0.004	1.50(-1) 0.002	1.49(-1) 0.001	1.49(-1)
$\delta = 1.7$	9.34(-2) 0.041	9.11(-2) 0.018	9.00(-2) 0.008	8.95(-2) 0.004	8.93(-2) 0.002	8.91(-2)
$\delta = 1.9$	3.54(-2) -0.058	3.68(-2) -0.041	3.79(-2) -0.026	3.86(-2) -0.015	3.90(-2) -0.009	3.93(-2)

TABLE 9. Example 2.1 with $D^\delta = D^\delta_{RL}$: scheme of [16, 17] with $(p, q) = (1, 0)$

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	5.39(-1) 0.102	5.02(-1) 0.099	4.69(-1) 0.100	4.38(-1) 0.100	4.08(-1) 0.100	3.81(-1)
$\delta = 1.3$	1.53(-1) 0.295	1.25(-1) 0.298	1.01(-1) 0.299	8.24(-2) 0.299	6.69(-2) 0.300	5.44(-2)
$\delta = 1.5$	3.96(-2) 0.491	2.82(-2) 0.496	2.00(-2) 0.498	1.41(-2) 0.499	1.00(-2) 0.499	7.08(-3)
$\delta = 1.7$	8.08(-3) 0.686	5.03(-3) 0.693	3.11(-3) 0.696	1.92(-3) 0.698	1.18(-3) 0.699	7.29(-4)
$\delta = 1.9$	7.66(-4) 0.873	4.18(-4) 0.887	2.26(-4) 0.893	1.22(-4) 0.897	6.54(-5) 0.898	3.51(-5)

TABLE 10. Example 2.2 with $D^\delta = D^\delta_{RL}$: scheme of [16, 17] with $(p, q) = (1, 0)$

4.4. **Spline-based scheme of** [14]**.** In [14] the authors approximate D^δ_{RL} by the spline-based approximation

$$D^\delta_{RL} u(x_j) \approx \frac{1}{h^\delta \Gamma(4-\delta)} \sum_{k=0}^{j+1} q_{jk} u_k, \tag{4.5}$$

where

$$\begin{aligned} q_{jk} &= a_{j-1,k} - 2a_{jk} + a_{j+1,k}, \quad \text{for} \quad k \le j-1, \\ q_{jj} &= -2a_{jj} + a_{j+1,j}, \\ q_{j,j+1} &= a_{j+1,j+1}, \end{aligned}$$

and

$$a_{jk} = \begin{cases} (j-k+1)^{3-\delta} - 2(j-k)^{3-\delta} + (j-k-1)^{3-\delta} & \text{if } k \le j-1, \\ 1 & \text{if } k = j. \end{cases}$$

This approximation was designed originally for a Riemann-Liouville derivative defined on $(-\infty, 1]$, viz.,

$$D^{\delta}_{RL,-\infty} g(x) := \left(\frac{d}{dx}\right)^2 \left[\frac{1}{\Gamma(2-\delta)} \int_{t=-\infty}^{x} (x-t)^{1-\delta} g(t)\, dt\right]$$

for $-\infty < x \le 1$. In [14, Theorem 2] it is proved that the approximation is formally second-order consistent if $u \in C^4(\mathbb{R})$ with $u^{(4)}(x) \equiv 0$ for $x \le 0$. We examine here how this approximation performs in the bounded domain $[0, 1]$.

Table 11 contains the results obtained when this scheme is used to solve Example 2.1. For every value of δ, there is no convergence as $N \to \infty$. Numerical results for Example 2.2 are presented in Table 12; similarly to the shifted Grünwald-Letnikov scheme, this spline-based scheme has order of convergence $\delta - 1$.

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	9.22(-1) 0.003	9.20(-1) -0.002	9.21(-1) -0.001	9.22(-1) -0.000	9.22(-1) -0.000	9.22(-1)
$\delta = 1.3$	8.32(-1) -0.012	8.40(-1) -0.005	8.43(-1) -0.002	8.44(-1) -0.001	8.45(-1) -0.001	8.45(-1)
$\delta = 1.5$	8.29(-1) -0.018	8.40(-1) -0.008	8.44(-1) -0.004	8.47(-1) -0.002	8.48(-1) -0.001	8.48(-1)
$\delta = 1.7$	8.76(-1) -0.022	8.89(-1) -0.010	8.95(-1) -0.005	8.98(-1) -0.002	9.00(-1) -0.001	9.01(-1)
$\delta = 1.9$	9.40(-1) -0.023	9.55(-1) -0.011	9.63(-1) -0.006	9.67(-1) -0.003	9.69(-1) -0.001	9.69(-1)

TABLE 11. Example 2.1 with $D^{\delta} = D^{\delta}_{RL}$: spline-based scheme [14]

	N=32	N=64	N=128	N=256	N=512	N=1024
$\delta = 1.1$	5.47(-1) 0.106	5.08(-1) 0.099	4.75(-1) 0.100	4.43(-1) 0.100	4.13(-1) 0.100	3.86(-1)
$\delta = 1.3$	1.55(-1) 0.296	1.26(-1) 0.298	1.03(-1) 0.299	8.36(-2) 0.299	6.79(-2) 0.300	5.52(-2)
$\delta = 1.5$	3.88(-2) 0.491	2.76(-2) 0.496	1.96(-2) 0.498	1.39(-2) 0.499	9.81(-3) 0.499	6.94(-3)
$\delta = 1.7$	7.01(-3) 0.682	4.37(-3) 0.691	2.71(-3) 0.696	1.67(-3) 0.698	1.03(-3) 0.699	6.35(-4)
$\delta = 1.9$	3.84(-4) 0.842	2.14(-4) 0.871	1.17(-4) 0.886	6.33(-5) 0.893	3.41(-5) 0.896	1.83(-5)

TABLE 12. Example 2.2 with $D^\delta = D^\delta_{RL}$: spline-based scheme [14]

4.5. **Proof of failure of shifted G-L scheme for Example 2.1.** In this section we prove rigorously that the shifted Grünwald-Letnikov scheme will fail to converge for a class of examples with polynomial solutions that includes Example 2.1.

In this section the solution of the boundary value problem is denoted by p to emphasize that here we discuss only polynomial solutions. To discretize the boundary value problem $D^\delta_{RL} p = f$ where $p(0)$ and $p(1)$ are given, we use the shifted Grünwald-Letnikov finite difference scheme

$$D^{\delta,N}_{GL,S} p_j = f_j \quad \text{for} \quad j = 1, 2, \dots, N-1, \tag{4.6a}$$

$$p_0 = p(0),\ p_N = p(1), \tag{4.6b}$$

where $D^{\delta,N}_{GL,S}$ is the approximation defined in (4.3). Denote by $A^\delta_{GL,S}$ the matrix associated with the scheme (4.6):

$$A^\delta_{GL,S} = \begin{pmatrix} -1 & 0\cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ w_2^{(\delta)} & w_1^{(\delta)} & w_0^{(\delta)} & & & & \\ w_3^{(\delta)} & w_2^{(\delta)} & w_1^{(\delta)} & w_0^{(\delta)} & & & \\ \vdots & \vdots & \vdots & \vdots & & \ddots & \\ w_N^{(\delta)} & w_{N-1}^{(\delta)} & \cdots & \cdots & \cdots & w_1^{(\delta)} & w_0^{(\delta)} \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & -1 \end{pmatrix}$$

Thus the approximation $\vec{p}_N := (p_0, p_1, \dots, p_N)^T$ defined by the scheme (4.6) is computed by solving the linear system

$$A^\delta_{GL,S} \vec{p}_N = \vec{f}, \tag{4.7}$$

with $\vec{f} = (-p(0), f_1, \ldots, f_{N-1}, -p(1))^T$. Here we have multiplied the boundary conditions by -1 to give all entries along the main diagonal of $A^{\delta}_{GL,S}$ the same sign.

For any mesh function w let $\|w\|_{\infty,d} = \max\{|w_i| : i = 0, 1, \ldots, N\}$ denote the discrete maximum norm of w. The notation

$$p - \vec{p}_N := (0, p(x_1) - p_1, \ldots, p(x_{N-1}) - p_{N-1}, 0)^T$$

is used to denote the vector of nodal errors.

We now show that when $p(0) \neq 0$, the shifted Grünwald-Letnikov scheme *cannot yield a positive order of convergence.*

Theorem 4.1. *Assume that the solution of the Dirichlet boundary value problem*

$$D^{\delta}_{RL} p(x) = f(x) \quad \text{for} \quad x \in (0,1), \quad p(0), p(1) \quad \text{given} \tag{4.8}$$

is the polynomial function $p(x) = \sum_{m=0}^{l} c_m x^m$ *with* $l \geq 0$ *and* $c_0 \neq 0$. *There do NOT exist positive constants* C *and* α, *which are independent of the mesh, such that the computed solution* $\vec{p}_N$ *of* (4.6) *satisfies*

$$\|p - \vec{p}_N\|_{\infty,d} \leq C h^{\alpha}. \tag{4.9}$$

P r o o f. Suppose the result is false, i.e., suppose that (4.9) is true.

For $j = 1, 2, \ldots, N-1$, the sum of all the elements of the j^{th} row of the difference scheme matrix $A^{\delta}_{GL,S}$ is, from [10, (2.8) and (2.9)] and [9, (1.2.8)],

$$\begin{aligned} h^{-\delta} \sum_{k=0}^{j+1} (-1)^k \binom{\delta}{k} = h^{-\delta} \sum_{k=0}^{j+1} \binom{k-\delta-1}{k} &= h^{-\delta} \binom{j+1-\delta}{j+1} \\ &= h^{-\delta} \frac{\Gamma(j-\delta+2)}{\Gamma(1-\delta)\Gamma(j+2)}. \end{aligned}$$

Consider the equation in the difference scheme that corresponds to $j = 1$ here; it states that

$$w_2^{(\delta)} p_N(0) + w_1^{(\delta)} p_N(h) + w_0^{(\delta)} p_N(2h) = f(h). \tag{4.10}$$

But

$$p_N(0) = c_0, \quad p_N(h) = c_0 + O(h) + O(h^{\alpha}), \quad p_N(2h) = c_0 + O(h) + O(h^{\alpha})$$

by the smoothness of p and the assumed bound (4.9), while

$$f(h) = \frac{c_0 h^{-\delta}}{\Gamma(1-\delta)} + O(h^{1-\delta})$$

like the calculation of f in Example 2.1. Substituting into (4.10) then taking only the highest-order terms (which will dominate as $h \to 0$), these equations yield, as $h \to 0$,

$$\frac{c_0 h^{-\delta}\Gamma(3-\delta)}{\Gamma(1-\delta)\Gamma(3)} = \frac{c_0 h^{-\delta}}{\Gamma(1-\delta)} + \text{ lower-order terms,}$$

– but this cannot be true as $\Gamma(3-\delta) \neq \Gamma(3)$. This contradiction implies our result. $\square$

Remark 4.1. A similar argument shows that Theorem 4.1 also holds true for the schemes of Sections 4.3 and 4.4. This negative result is born out by Tables 9 and 11.

5. **Conclusions**

In this paper we considered simple two-point boundary value problems whose highest-order derivative is either a Riemann-Liouville or a Caputo fractional derivative. Approximate solutions to these problems were computed by some standard different schemes from the research literature. Our purpose was to explore how well standard schemes behave when applied to problems with polynomial solutions (and consequently non-smooth right-hand sides) and problems with smooth right-hand sides (and consequently non-smooth solutions). Throughout the paper we use the discrete maximum norm – the most natural norm for finite difference methods.

The theoretical background for most schemes is a bound on the formal consistency error (i.e., the order of consistency attained under the strong hypothesis that the solution is smooth enough to permit Taylor series expansions or to induce fast decay at infinity of the Fourier transform of the solution), but it is not clear theoretically that the same order of convergence is achieved when the scheme is applied in practice. Our numerical experiments are designed to give practical information about the true behaviour of these schemes.

For a Caputo fractional derivative, we tested two schemes. These schemes yielded orders of convergence equal to their formal orders of consistency for a polynomial solution, but attained only first-order convergence when the solution was nonsmooth despite one of the schemes having formal second-order consistency.

The Riemann-Liouville fractional derivative is more challenging. The well-known L2 scheme was first-order accurate for our polynomial solution but the order of convergence deteriorated in the other example. The other schemes that we tested all failed to converge for the polynomial solution example, and were $O(h^{\delta-1})$ accurate for the other example.

When the solution $u(x)$ is a polynomial, we proved rigorously that the shifted Grünwald-Letnikov difference scheme (and some other schemes) fail to converge if $u(0) \neq 0$. In a subsequent paper we shall examine how one can improve the order of convergence of finite difference methods when faced with situations like this.

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