

Analysis and numerical solution of a Riemann-Liouville fractional derivative two-point boundary value problem

Natalia Kopteva · Martin Stynes

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Abstract A two-point boundary value problem is considered on the interval $[0, 1]$, where the leading term in the differential operator is a Riemann-Liouville fractional derivative of order $2 - \delta$ with $0 < \delta < 1$. It is shown that any solution of such a problem can be expressed in terms of solutions to two associated weakly singular Volterra integral equations of the second kind. As a consequence, existence and uniqueness of a solution to the boundary value problem are proved, the structure of this solution is elucidated, and sharp bounds on its derivatives (in terms of the parameter δ) are derived. These results show that in general the first-order

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The second author is the Corresponding Author.

Natalia Kopteva

Department of Mathematics and Statistics, University of Limerick, Ireland.

E-mail: natalia.kopteva@ul.ie

Martin Stynes

Beijing Computational Science Research Center, Haidian District, Beijing 100193, China.

Tel.: +86-10-56981801, Fax: +86-10-56981700. E-mail: m.stynes@csrc.ac.cn

derivative of the solution will blow up at $x = 0$, so accurate numerical solution of this class of problems is not straightforward. The reformulation of the boundary problem in terms of Volterra integral equations enables the construction of two distinct numerical methods for its solution, both based on piecewise-polynomial collocation. Convergence rates for these methods are proved and numerical results are presented to demonstrate their performance.

Keywords Fractional differential equation · Riemann-Liouville fractional derivative · boundary value problem · weakly singular Volterra integral equation · collocation method

Mathematics Subject Classification (2000) 65L10

1 Introduction

At present there is much active research into the design and analysis of numerical methods for differential equations containing fractional-order derivative because these derivatives are useful in modelling certain physical processes; see the discussion and references in [5]. In particular, numerical methods for two-point boundary value problems involving Riemann-Liouville derivatives have been examined in many papers. Despite this high level of activity, existence/uniqueness/regularity results for this class of problems have been confined to problems where the differential operator does not include a convective term (see [4, 5] and their references).

To analyse rigorously the convergence of any numerical method for Riemann-Liouville fractional-derivative boundary value problems, one needs information about the existence, uniqueness and regularity of the solution. The pointwise regularity of solutions to Riemann-Liouville boundary value problems that include a

convective term is still an open question, and as a consequence there are currently no rigorous convergence results for finite difference or collocation methods for this class of problems.

In the present paper we make two contributions to filling this gap in the literature. We prove existence, uniqueness and regularity (in a pointwise sense) for a class of Riemann-Liouville two-point boundary problems that permits convective terms, and present two efficient collocation methods for their solution for which we obtain rigorous error bounds.

The structure of the paper is as follows. Section 1 presents the fractional-derivative two-point boundary value problem that we study. In Section 2 it is shown that the solution of this problem is equivalent to the solution of a pair of weakly singular Volterra integral equations of the second kind. This enables us to prove existence and uniqueness of a solution to the original boundary value problem. Then in Section 3 we construct and analyse two numerical methods for solving the boundary value problem that are based on Volterra integral equation reformulations of the problem.

Notation. Let $\mathbb{N} = \{1, 2, \dots\}$ denote the set of natural numbers. We use the standard notation $C^k(I)$ to denote the space of real-valued functions whose derivatives up to order k are continuous on an interval I , and write $C(I)$ for $C^0(I)$. For each $g \in C[0, 1]$, set $\|g\| = \max_{x \in [0, 1]} |g(x)|$. The Lebesgue space $L_1[0, 1]$ is used occasionally.

In several inequalities C denotes a generic constant that depends on the data of the boundary value problem (3) and possibly on the mesh grading but is independent of the mesh diameter when (3) is solved numerically; note that C can take different values in different places.

1.1 Basic definitions

For $n = 1, 2, \dots$ we 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

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

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

Let $\mu > 0$. For all $g \in L_1[0, 1]$, as in [3] define the *Riemann-Liouville fractional integral operator* of order μ by

$$(J^\mu g)(x) = \frac{1}{\Gamma(\mu)} \int_{t=0}^x (x-t)^{\mu-1} g(t) dt \quad \text{for } 0 \leq x \leq 1. \quad (1)$$

We shall make frequent use of the property [3, Theorem 2.2] $J^{\mu_1 + \mu_2} g = J^{\mu_1} J^{\mu_2} g$ for all $\mu_1, \mu_2 \geq 0$ and $g \in L_1[0, 1]$.

Let m be a positive integer. Let $\delta \in (0, 1)$. For any suitable function g , the *Riemann-Liouville fractional derivative* $D^{m-\delta}$ is defined [3, Definition 2.2] by

$$D^{m-\delta} g(x) = \left(\frac{d}{dx} \right)^m (J^\delta g)(x) \quad \text{for } 0 < x \leq 1, \quad (2)$$

If $g \in A^m[0, 1]$, then this derivative is well defined. Note that if one sets $\delta = 0$ and $m = 1$, then the Riemann-Liouville derivative $D^1 \equiv D$ becomes the classical differential operator d/dx .

1.2 The boundary value problem

In this paper we consider the Riemann-Liouville two-point boundary value problem

$$Lu := -D^{2-\delta}u + (bu)' + cu = f \quad \text{on } (0, 1), \quad (3a)$$

$$u(0) = 0, \quad (3b)$$

$$\alpha u(1) + \beta u'(1) = \gamma, \quad (3c)$$

where $0 < \delta < 1$, $b \in C[0, 1] \cap C^1(0, 1)$, c and $f \in C[0, 1]$, and $\alpha, \beta, \gamma \in \mathbb{R}$ are given constants. In later sections further hypotheses will be placed on these functions and constants as they are needed. A discussion of anomalous diffusion processes in nature that motivate the study of this boundary value problem is given in [5, Section 1.1].

The problem (3) is well-posed: in Theorem 2 we give necessary and sufficient conditions for existence and uniqueness of a solution to (3), and in Theorem 3 we give sufficient conditions on the data of (3) to guarantee existence and uniqueness of that solution.

The choice of the homogeneous Dirichlet boundary condition $u(0) = 0$ in (3b) is motivated by the following example and discussion.

Example 1 Consider $-D^{2-\delta}u = 1$ on $(0, 1)$, with the boundary conditions (3b).

The general solution of this differential equation is, by [3, Example 2.4],

$$u(x) = -\frac{x^{2-\delta}}{\Gamma(1-\delta)} + c_1 x^{1-\delta} + c_2 x^{-\delta}$$

for some constants c_1 and c_2 . The boundary condition $u(0) = 0$ forces $c_2 = 0$. This is desirable as $c_2 \neq 0$ would imply $u \notin C[0, 1]$, thereby making the problem much

more difficult to analyse. Then the boundary condition at $x = 1$ will determine the value of c_1 . In general one has $c_1 \neq 0$, so $u \in C[0, 1] \cap C^1(0, 1]$ but $u \notin C^1[0, 1]$. In fact $u'(x)$ blows up at $x = 0$. One has $u \in A^1[0, 1]$ but $u \notin A^2[0, 1]$.

Furthermore, in our analysis we shall consider only solutions u for which $D^{1-\delta}u \in C[0, 1]$, but an elementary argument [8, Lemma 3.1] shows that this property forces $u(0) = 0$.

In (3) the convection term $(bu)'$ is written in conservative form for our later convenience. The nonconservative form bu' can be rewritten as $(bu)' - b'u$ to fit into this framework.

2 Analysis of the boundary value problem

Our aim here is to reformulate (3) in terms of Volterra integral equations in order to show existence, uniqueness and regularity of a solution to (3), and furthermore to facilitate its efficient numerical solution. A related reformulation was used in [7], where a Caputo boundary value problem was rewritten in terms of the continuous variable u' , but in (3)—as we saw in Example 1—one may have $u' \notin C[0, 1]$, which would not fit with the standard Volterra theory in [1] so a different reformulation will be necessary here. Fundamentally, the Riemann-Liouville boundary value problem (3) is less well behaved than the analogous Caputo problem of [7] and requires more work for its satisfactory analysis and accurate numerical solution.

2.1 Equivalence of (3) to Volterra integral equations

The first result is a generalisation of Example 1.

Lemma 1 Let $g \in L_1[0, 1]$. Then the general solution of the differential equation

$D^{2-\delta}r = g$ on $(0, 1)$ is given by

$$r(x) = (J^{2-\delta}g)(x) + c_1x^{1-\delta} + c_2x^{-\delta} \quad (4)$$

for arbitrary constants c_1 and c_2 . If in addition $r(0) = 0$, then $c_2 = 0$.

Proof The function $J^{2-\delta}g$ is a particular solution of $D^{2-\delta}r = g$ by [3, Theorem 2.14]. Equation (4) now follows from the discussion in [3, p.54]. Next, it is easy to see from the definition of $J^{2-\delta}$ that $(J^{2-\delta}g)(x) \rightarrow 0$ as $x \rightarrow 0$. Consequently one can have $r(0) = 0$ in (4) only if $c_2 = 0$. \square

Assume that $u \in A^1[0, 1]$. Rearranging (3a) and applying Lemma 1, we have

$$u(x) = \left(J^{2-\delta}((bu)' + cu - f) \right)(x) + c_1x^{1-\delta}$$

for some constant c_1 . But $u(0) = 0$ so one can integrate $J^{2-\delta}(bu)'$ by parts to get

$$u(x) = J^{1-\delta}(bu)(x) + J^{2-\delta}(cu)(x) - J^{2-\delta}f(x) + c_1x^{1-\delta}. \quad (5)$$

Now split (5) into two independent weakly singular Volterra integral equations of the second kind, so that $u = c_1v + w$:

$$v(x) = J^{1-\delta}(bv)(x) + J^{2-\delta}(cv)(x) + x^{1-\delta} \quad (6a)$$

and

$$w(x) = J^{1-\delta}(bw)(x) + J^{2-\delta}(cw)(x) - J^{2-\delta}f(x) \quad (6b)$$

for $0 \leq x \leq 1$.

Example 2 If $b = \lambda \in \mathbb{R}$ is constant and $c \equiv 0$, then one can compute (see the derivation of (21) later and [9, (1.82)])

$$v(x) = x^{1-\delta} \Gamma(2-\delta) E_{1-\delta, 2-\delta}(\lambda x^{1-\delta}) \quad \text{and} \quad v'(x) = x^{-\delta} \Gamma(2-\delta) E_{1-\delta, 1-\delta}(\lambda x^{1-\delta}),$$

where the two-parameter Mittag-Leffler function E is defined by

$$E_{\mu, \theta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\mu k + \theta)} \quad \text{for } \mu, \theta, z \in \mathbb{R} \text{ with } \mu > 0. \quad (7)$$

This function is discussed in [3, 9]. These formulas, combined with known properties of the Mittag-Leffler function, imply that for any $\lambda \in \mathbb{R}$ one has $v(x) > 0$ and $v'(x) > 0$ for $x > 0$, and $v'(0^+) = +\infty$.

To discuss the solutions of (6), we introduce a family of spaces that is often used (e.g., in [2, 7]) in the analysis of weakly singular integral equations.

For $q \in \{0, 1, 2, \dots\}$ and $-\infty < \nu < 1$ with ν not an integer, let $C^{q, \nu}(0, 1]$ denote the space of functions $y \in C[0, 1] \cap C^q(0, 1]$ such that

$$|y^{(k)}(x)| \leq C \left[x^{(1-\nu)-k} + 1 \right] \quad \text{for } k = 0, 1, \dots, q \text{ and } x \in (0, 1]. \quad (8)$$

In particular, $C^{0, \nu}(0, 1] = C[0, 1]$.

Theorem 1 *Assume that $b \in C^{q, \delta}(0, 1]$ and $c \in C^{q-1, \delta}(0, 1]$ for some $q \in \mathbb{N}$. Then (6a) has a unique solution $v \in C^{q, \delta}(0, 1]$ with $v(0) = 0$.*

Assume also that

$$\begin{cases} f \in L_p[0, 1] \text{ for some } p > 1/(1-\delta) & \text{if } q = 1, \\ f \in C^{q-1, \delta}(0, 1] & \text{if } q > 1. \end{cases}$$

Then (6b) has a unique solution $w \in C^{q, \delta}(0, 1] \cap C^{2, \delta-1}(0, 1] \subset C^1[0, 1]$ with $w(0) = 0$.

Proof Existence and uniqueness of a solution $v \in C^{q,\delta}(0,1]$ for (6a) is a straightforward extension of [2, Remark 3] (cf. [7, Lemma 2.1]): observe that the forcing function $x^{1-\delta}$ of (6a) lies in $C^{q,\delta}(0,1]$, $v \mapsto bv$ is a bounded mapping from $C^{q,\delta}(0,1]$ to itself by [2, Lemma 2.1], $J^{1-\delta} : C^{q,\delta}(0,1] \rightarrow C^{q,\delta}(0,1]$ is compact [2, Lemma 2.2] and similarly $v \mapsto J^{2-\delta}(cv) = J^{1-\delta}J(cv)$ defines a compact operator $C^{q,\delta}(0,1] \rightarrow C^{q,\delta}(0,1]$. As we now have $v \in C[0,1]$, the property $v(0) = 0$ follows quickly from (6a).

For (6b), consider first the case $q = 1$. Then $f \in L_p[0,1]$ with $p > 1/(1-\delta)$ implies $J^{1-\delta}f \in C[0,1]$ by [3, Theorem 2.6]. Consequently $J^{2-\delta}f = J(J^{1-\delta}f)$ is in $C^1[0,1] \subset C^{1,\delta}(0,1]$. In the case $q > 1$, $f \in C^{q-1,\delta}(0,1]$ implies $Jf \in C^{q,\delta}(0,1]$ and hence $J^{2-\delta}f = J^{1-\delta}(Jf)$ is in $C^{q,\delta}(0,1]$ by [2, Lemma 2.2]. Thus for all $q \in \mathbb{N}$ one has $J^{2-\delta}f \in C^{q,\delta}(0,1]$.

Now, as for (6a), we get $w \in C^{q,\delta}(0,1] \subset C[0,1]$. But $J^{1-\delta}f \in C[0,1]$ implies $J^{2-\delta}f(0) = 0$ and hence $w(0) = 0$ from (6b). Using this property, integrate (6b) by parts, obtaining $w = J^{2-\delta}(cw + (bw)' - f)$; this can be differentiated to yield

$$w' = J^{1-\delta}(cw + (bw)' - f) = J^{1-\delta}(bw') + J^{1-\delta}(cw + b'w - f) \quad (9)$$

which is a Volterra integral equation in w' where $J^{1-\delta}(cw + b'w - f) \in C[0,1]$ is regarded as given. Thus invoking [7, Lemma 2.1] we get $w' \in C^{1,\delta}(0,1]$. This implies that $w \in C^{2,\delta-1}(0,1]$, and functions in this space can be extended to lie in $C^1[0,1]$. \square

Above we derived (6) from (3a) and (3b). Now we proceed in the opposite direction to show the equivalence of these two formulations.

Let v and w be the unique solutions of (6a) and (6b) that are guaranteed by Theorem 1. For any c_1 , the function $u := w + c_1v$ satisfies (3a) by (6a) and (6b),

as $D^{2-\delta} = DD^{1-\delta}$ by the definition (2), and $D^r J^r$ (any $r > 0$) is the identity operator by [3, Theorem 2.14]. Furthermore $u(0) = 0$ since $v(0) = w(0) = 0$ from Theorem 1.

We can now clarify when one has existence and uniqueness of a solution to (3).

Theorem 2 *Assume the same hypotheses as Theorem 1. Let v and w be the unique solutions of (6) that are provided by that theorem.*

1. *If $\alpha v(1) + \beta v'(1) \neq 0$, then (3) has a unique solution*

$$u = w + c_1 v \in C^{q,\delta}(0, 1], \text{ where } c_1 := \frac{\gamma - \alpha w(1) - \beta w'(1)}{\alpha v(1) + \beta v'(1)}. \quad (10)$$

2. *If $\alpha v(1) + \beta v'(1) = 0$, then (3) has either no solution or infinitely many solutions.*

Proof As we have seen, (3a) and (3b) are equivalent to (6). Thus existence of a unique solution of (3) is equivalent to having a unique choice of c_1 in $u := w + c_1 v$ that enables u to satisfy the remaining boundary condition $\alpha u(1) + \beta u'(1) = \gamma$ of (3c).

If $\alpha v(1) + \beta v'(1) \neq 0$, then since $u = w + c_1 v$ it is clear that $\alpha u(1) + \beta u'(1) = \gamma$ if and only if c_1 is chosen according to (10).

On the other hand, suppose that $\alpha v(1) + \beta v'(1) = 0$. Then there is no solution to (3c) if $\alpha w(1) + \beta w'(1) \neq \gamma$, while if $\alpha w(1) + \beta w'(1) = \gamma$ then $u = w + c_1 v$ is a solution of (3c) for any choice of $c_1 \in \mathbb{R}$. \square

2.2 Sufficient conditions for existence and uniqueness of a solution to (3)

In this section we place conditions on the data of (3) that will imply

$$\alpha v(1) + \beta v'(1) > 0. \quad (11)$$

Then Theorem 2 yields existence and uniqueness of a solution to (3).

At various points in this section, we shall assume one or more of the inequalities

$$c \geq 0 \quad \text{on } [0, 1], \quad (12a)$$

$$b' + c \geq 0 \quad \text{on } [0, 1]. \quad (12b)$$

$$\alpha \geq 0, \beta \geq 0 \quad \text{and} \quad \alpha + \beta > 0 \quad \text{in (3c)}. \quad (12c)$$

Conditions such as these are commonly assumed in classical second-order differential equations to ensure that the differential operator L and its formal adjoint satisfy a maximum principle.

Lemma 2 *Assume condition (12a), $b \in C^{1,\delta}(0, 1]$ and $c \in C^{0,\delta}(0, 1]$. Then $v(x) > 0$ for all $x \in (0, 1]$.*

Proof Integrate by parts using $v(0) = 0$ to write (6a) as

$$v(x) = J^{2-\delta}(cv + (bv)')(x) + x^{1-\delta} \quad \text{for } 0 \leq x \leq 1. \quad (13)$$

Differentiating and using $DJ^{2-\delta} = DJ^1J^{1-\delta} = J^{1-\delta}$, we get

$$v'(x) = J^{1-\delta}(cv + (bv)')(x) + (1-\delta)x^{-\delta} \quad \text{for } 0 < x < 1. \quad (14)$$

But $v \in C^{1,\delta}(0, 1]$ by Theorem 1, so $|cv + (bv)'(x)| = |((c + b')v + bv)'(x)| \leq Cx^{-\delta}$ and it follows by a standard estimate for Euler's Beta function [3, Theorem D.6] that $|J^{1-\delta}(cv + (bv)')(x)| = O(x^{1-2\delta})$. Consequently (14) implies that $v'(x) > 0$ for all x sufficiently close to $x = 0$.

Now suppose that the conclusion of the lemma is false. Set $x^* = \inf\{x \in (0, 1] : v(x) \leq 0\}$. As $v(0) = 0$ and $v'(x) > 0$ near $x = 0$, one has $0 < x^* \leq 1$. Furthermore, by continuity $v(x^*) = 0$.

Applying $D^{1-\delta}$ to (6a) gives

$$D^{1-\delta}v(x) - (bv)(x) - \int_{t=0}^x c(t)v(t) dt = \Gamma(2-\delta) \text{ on } (0, 1], \quad (15)$$

since $J^{2-\delta} = J^{1-\delta}J$, $D^{1-\delta}J^{1-\delta} = I$ and $D^{1-\delta}x^{1-\delta} = \Gamma(2-\delta)$ by Theorem 2.2, Theorem 2.14 and Example 2.4 of [3]. At $x = x^*$, as $v(x^*) = 0$ the equation (15) becomes

$$\begin{aligned} \Gamma(2-\delta) + \int_{t=0}^{x^*} c(t)v(t) dt &= D^{1-\delta}v(x^*) \\ &= \frac{d}{dx} \left(\frac{1}{\Gamma(\delta)} \int_{t=0}^x (x-t)^{\delta-1}v(t) dt \right) \Big|_{x=x^*} \\ &= \frac{\delta-1}{\Gamma(\delta)} \int_{t=0}^{x^*} (x^*-t)^{\delta-2}v(t) dt, \end{aligned}$$

as can be seen by integrating by parts before and after applying d/dx , and using the property $|v(t)| \leq C(x^* - t)$ for $0 \leq t \leq x^*$ which follows from $v(x^*) = 0$ and $v \in C[0, 1] \cap C^q(0, 1]$. But $\delta - 1 < 0$ and $v(t) > 0$ for $0 < t < x^*$, so the right-hand side of the equation is negative while the left-hand side is positive by (12a). From this contradiction we infer that the lemma is true. \square

Lemma 3 *Assume conditions (12a) and (12b), $b \in C^{1,\delta}(0, 1]$ and $c \in C^{0,\delta}(0, 1]$. Then $v'(x) > 0$ for all $x \in (0, 1]$.*

Proof Set $s = v'$. We saw in the proof of Lemma 2 that $s(x) > 0$ for all x near $x = 0$.

Applying $D^{1-\delta}$ to (14) yields (like the derivation of (15))

$$D^{1-\delta}s(x) = [bs + (b' + c)v](x) \quad \text{on } (0, 1]. \quad (16)$$

Suppose that the conclusion of the lemma is false. Set $x^* = \inf\{x \in (0, 1] : s(x) \leq 0\}$. Then $x^* \in (0, 1]$ since $s(x) > 0$ near $x = 0$. We now derive a contradiction in (16)

at $x = x^*$ by imitating the proof of Lemma 2, but with the argument modified to handle the complication that $s(x)$ blows up as $x \rightarrow 0$. Choose $\bar{x} \in (0, x^*)$. Then

$$\begin{aligned} D^{1-\delta}s(x)\Big|_{x=x^*} &= \frac{d}{dx} \left(\frac{1}{\Gamma(\delta)} \int_{t=0}^{\bar{x}} (x-t)^{\delta-1} s(t) dt \right) \Big|_{x=x^*} \\ &\quad + \frac{d}{dx} \left(\frac{1}{\Gamma(\delta)} \int_{t=\bar{x}}^x (x-t)^{\delta-1} s(t) dt \right) \Big|_{x=x^*} \\ &= \frac{\delta-1}{\Gamma(\delta)} \left[\int_{t=0}^{\bar{x}} (x^*-t)^{\delta-2} s(t) dt + \int_{t=\bar{x}}^{x^*} (x^*-t)^{\delta-2} s(t) dt \right]; \end{aligned}$$

here the differentiation of the first integral is routine while for the second we integrate by parts, then differentiate, then integrate by parts again. As $s(x) > 0$ on $(0, x^*)$ it follows that $D^{1-\delta}s(x)\Big|_{x=x^*} < 0$. But this inequality contradicts (16) at $x = x^*$ since $s(x^*) = 0$ by the definition of x^* and $[(b'+c)v](x^*) > 0$ by Lemma 2 and (12b). This concludes the proof. \square

We come now to the main result of this section.

Theorem 3 [Existence and uniqueness of a solution to the Riemann-Liouville boundary value problem (3)] *Assume the hypotheses of Theorem 1. Assume all three conditions in (12). Then (3) has a unique solution $u \in C^{q,\delta}(0, 1]$.*

Proof Lemmas 2 and 3 imply that $\alpha z(1) + \beta z'(1) > 0$ since $\alpha \geq 0$, $\beta \geq 0$ and $\alpha + \beta > 0$. Now Theorem 2 gives the desired result. \square

Remark 1 In the case where (3) has a Dirichlet boundary condition at $x = 1$ (i.e., when $\beta = 0$), Lemma 3 is no longer needed and consequently the assumption (12b) can be removed from Theorem 3. Similarly, one does not need the condition (12b) in the remainder of the paper when $\beta = 0$.

Note that $u \in C^{q,\delta}(0, 1]$ gives the useful pointwise bound

$$|u^{(i)}(x)| \leq Cx^{1-i-\delta} \quad \text{for } i = 1, 2, \dots, q \text{ and } 0 < x \leq 1 \quad (17)$$

from the definition of the space $C^{q,\delta}(0,1]$.

Example 1 shows that this bound is sharp. Nevertheless the bound does not give us a complete picture of the regularity of u , because $D^{2-\delta}g$ is not defined for all functions g that satisfy (17) yet $D^{2-\delta}u$ is defined (it appears in (3a)). Remark 2 will shed more light on the properties of u , but first we derive a technical result that will prove useful in discussing u here and in constructing a numerical method for solving (3) in Section 3.1.

Remark 2 [A further comment on the regularity of u] Example 1 shows that u may not lie in $A^2[0,1]$, but the differential equation (3a) that u satisfies includes the term $D^{2-\delta}u$ which is frequently perceived to be well defined only when $u \in A^2[0,1]$. This anomaly arises because u may have a singular component that lies outside $A^2[0,1]$ but is annihilated by the differential operator—for instance, the $x^{1-\delta}$ term in Example 1.

The decomposition of Theorem 2, stating that

$$u(x) = w(x) + c_1 v(x),$$

illustrates this structure. For Theorem 1 tells us that $w \in C^{2,\delta-1}[0,1]$, and it is straightforward to check that $C^{2,\delta-1}[0,1] \subset A^2[0,1]$, while v lies in $C^{q,\delta}(0,1]$ so in general $v \notin C^1[0,1]$ and therefore $v \notin A^2[0,1]$. But v satisfies the homogeneous analogue $Lv = 0$ of (3a): for, applying $D^{2-\delta}$ to (13), we get $D^{2-\delta}v = cv + (bv)'$, as desired.

Remark 3 [Existence and uniqueness for a Caputo two-point boundary value problem]

In [7] a result similar to the analysis of Sections 2.1 and 2.2 was obtained for a related two-point boundary value problem where the Riemann-Liouville derivative

in (3a) is replaced by a Caputo derivative: it was shown that the solution of the original problem can be expressed as an integral of a linear combination of the solutions to two weakly singular Volterra integral equations. One can easily deduce from the proof of that equivalence an existence and uniqueness result for the Caputo problem that is analogous to Theorem 3. Furthermore, this result requires (in the notation of [7]) only $\alpha_0 \geq 0$ instead of the more restrictive hypothesis $\alpha_0 \geq 1/(1 - \delta)$ that was used throughout that paper.

3 Two numerical methods for solving (3)

In this section we present and analyse two numerical methods for solving (3) numerically for u in an efficient way. Both methods are based on the representation

$$u = w + c_1 v \tag{18}$$

of Theorem 2. Thus w, v and c_1 need to be computed numerically.

In both methods, the solution of (3) is reduced to solving an independent pair of weakly singular Volterra integral equations. This is done by employing the collocation method of [7], which uses piecewise polynomials of degree $m - 1$ on a graded mesh; for completeness this method is described in detail in the Appendix below. We assume in Section 3 that the mesh grading parameter ρ that is defined in the Appendix satisfies $\rho \geq m/(1 - \delta)$ and that N , the number of mesh intervals, is sufficiently large, so that the error bounds from the Appendix can be invoked.

We assume that the functions b, c, f of (6) lie in $C^{q, \delta}(0, 1]$ with $q \geq m + 1$. The analyses of our numerical methods rely heavily on [6]. One should however note a difference between our definition of the space $C^{q, \delta}(0, 1]$ in (8) and the corresponding definition in [6, equation (2.2)], where an extra logarithmic factor appears; thus

our functions are slightly better behaved than those of [6]. An inspection of the arguments of [6] shows readily that if the logarithmic factor is removed from the definition of $C^{q,\delta}(0,1]$, this will remove all logarithmic factors from the subsequent analysis. Consequently the error bounds from [6] that we quote below have had a factor $\ln N$ removed wherever it appeared.

Furthermore, the collocation method of [6] uses a transformation of the independent variable, but its analysis remains valid for the special case where this transformation is the identity mapping (see [6, Remark 5.2]), and this special case is the method described in our Appendix.

Remark 4 In the special case where $b, c, f \in C^q[0,1] \subset C^{q,\delta}(0,1]$ with $q \geq m+1$, one can obtain similar convergence results more simply from [7, Corollaries 3.1 and 3.2].

In the error estimates of Section 3, the generic constants C depend on the choice of collocation parameters $\{c_j\}$ and on the mesh grading ρ , but are independent of the mesh diameter h .

3.1 Method I: singularity subtraction

In (18) we need to deal with v and w , but Theorem 2 reveals that v is worse behaved than w . We shall modify v by subtracting off the weak singularity that $v(x)$ has at $x=0$ before applying a numerical method from [7].

Set $W = w'$. Then, since $w(0) = 0$, one can write (9) as

$$W(x) - J^{1-\delta} \left(bW + (c+b') \int_0^{(\cdot)} W \right) (x) = -J^{1-\delta} f(x) \quad (19)$$

This Volterra equation has the same form as [7, (2.4)] so the collocation method and convergence analysis of [7] can be used in (19) to solve for W .

One cannot apply the same idea directly to v because $v' \notin C[0, 1]$. Thus we first subtract from v its weak singularity at $x = 0$. Set $\lambda = b(0)$. Retaining only the most significant terms from (6a), let v_0 be the solution of the Volterra equation

$$v_0(x) = J^{1-\delta}(\lambda v_0)(x) + x^{1-\delta} \quad \text{for } 0 \leq x \leq 1. \quad (20)$$

We derive an explicit formula for v_0 . Applying $D^{1-\delta}$ to (20) yields $D^{1-\delta}v_0 = \lambda v_0 + \Gamma(2-\delta)$, where we used [3, Example 2.4] to evaluate $D^{1-\delta}x^{1-\delta}$. One also has $v_0(0) = 0$ from (20). By [3, Theorem 7.2] the solution of this initial-value problem is

$$v_0(x) = \begin{cases} x^{1-\delta} & \text{if } \lambda = 0, \\ \frac{\Gamma(2-\delta)}{\lambda} \left[E_{1-\delta,1}(\lambda x^{1-\delta}) - 1 \right] = x^{1-\delta} \Gamma(2-\delta) E_{1-\delta,2-\delta}(\lambda x^{1-\delta}) & \text{if } \lambda \neq 0. \end{cases} \quad (21)$$

by elementary manipulations of the series for E . One can verify easily that $v_0 \in C^{q,\delta}(0, 1]$.

Set

$$s = v - v_0 \text{ and } S = s'. \quad (22)$$

Note that $s(0) = 0$. Subtracting (20) from (6a), we obtain

$$s = J^{2-\delta}(cv) + J^{1-\delta}(bv - \lambda v_0) = J^{2-\delta}(cv + (bv - \lambda v_0)')$$

after an integration by parts. Rearranging, this becomes

$$s = J^{2-\delta}((bs)' + cs + (b - \lambda)v_0' + (c + b')v_0)$$

Set $S = s'$ and differentiate to get

$$S(x) - J^{1-\delta} \left(bS + (c + b') \int_0^{(\cdot)} S \right) (x) = J^{1-\delta} ((b - \lambda)v_0' + (c + b')v_0) (x). \quad (23)$$

Recalling that $\lambda = b(0)$ and $J^{1-\delta}$ maps $C^{q,\delta}(0, 1]$ to itself by [2, Lemma 2.2], one can see easily that the right-hand sides of (19) and (23) lie in $C^{q,\delta}(0, 1]$. Thus (19) and (23) have exactly the same form and regularity as the integral equation that was studied in [7] (see equation (2.4) there) and solved numerically using the iterated collocation method on a graded mesh of diameter h with piecewise polynomials of degree $m - 1 \geq 0$ lying in the space S_{m-1}^{-1} defined in (35), where the value of m is chosen by the user; a full description of this method is given in the Appendix below.

Write W_h^{it} and S_h^{it} for the computed solutions of (19) and (23) respectively.

Set

$$w_h(x) = \int_0^x W_h^{it}(t) dt \quad \text{and} \quad s_h(x) = \int_0^x S_h^{it}(t) dt \quad \text{for } x \in [0, 1]. \quad (24)$$

Lemma 4 *There exists a constant C such that*

$$\|w - w_h\| + \|W - W_h^{it}\| + \|s - s_h\| + \|S - S_h^{it}\| \leq C \left(Kh^m + h^{m+1-\delta} \right), \quad (25)$$

where the quantity K is defined in (44).

Proof The desired bounds for W_h^{it} and S_h^{it} are immediate from (48). The bound on $\|w - w_h\| + \|s - s_h\|$ then follow from the definitions of W and S . \square

Finally, we can compute an accurate approximation of u .

Theorem 4 *Assume both conditions in (12). Assume also that $\alpha \geq 0$, $\beta \geq 0$ and $\alpha + \beta > 0$ in (3c). Set $V_h = S_h^{it} + v_0'$ and $v_h(x) = \int_0^x V_h = s_h(x) + v_0(x)$ for $x \in [0, 1]$.*

Set

$$c_{1,h} = \frac{\gamma - \alpha w_h(1) - \beta W_h^{it}(1)}{\alpha v_h(1) + \beta V_h(1)} \quad (26)$$

and

$$u_h(x) = w_h(x) + c_{1,h}v_h(x) \quad \text{for } x \in (0, 1]. \quad (27)$$

Then for h sufficiently small, the quantity $c_{1,h}$ is well defined by (26) and

$$\|u - u_h\| \leq C \left(Kh^m + h^{m+1-\delta} \right) \quad (28)$$

for some constant C .

Proof First, Lemmas 2 and 3 and the hypotheses on α and β imply that $\alpha v(1) + \beta v'(1) > 0$. Now $v' - V_h = (S + v'_0) - (S_h^{it} + v'_0) = S - S_h^{it}$ and $v - v_h = s - s_h$, so by Lemma 4 one has

$$\|V - V_h\| + \|v - v_h\| \leq C \left(Kh^m + h^{m+1-\delta} \right). \quad (29)$$

This inequality ensures that the denominator of (26) is positive for h sufficiently small, and thus $c_{1,h}$ is well defined. Furthermore, Lemma 4 and (29) imply that $|c_1 - c_{1,h}| \leq C \left(Kh^m + h^{m+1-\delta} \right)$ and that (28) holds true, on recalling that $u = w + c_1v$ and $u_h = w_h + c_{1,h}v_h$. \square

3.2 Method II: direct solution of (6)

In this section we discuss an alternative numerical method for solving (18). It is based on computing approximations of v and w directly from (6)—i.e., unlike Section 3.1, approximations of v and w are not constructed from approximations of v' and w' .

Observe that $x^{1-\delta} = J^{1-\delta}(\Gamma(2-\delta))$ and consequently both Volterra equations in (6) have the form

$$r - J^{1-\delta} \left(br + \int (cr) \right) = J^{1-\delta} g,$$

where $J^{1-\delta}g$ is known and lies in $C^{q,\delta}(0, 1]$. This integral equation is almost identical to [7, (2.4)]: the only difference is that in [7] one has $c(x)\int_0^x r$ instead of $\int_0^x (cr)$. This minor change in the lowest-order term does not affect the analysis of [7]. Thus we can again use the iterated collocation method from our Appendix to solve (6a) and (6b) on a graded mesh of diameter h with piecewise polynomials of degree $m-1 \geq 0$, where m is chosen by the user.

Theorem 5 *Assume both conditions in (12). Assume also that $\alpha \geq 0$, $\beta \geq 0$ and $\alpha + \beta > 0$ in (3c). Let \tilde{v}_h and \tilde{w}_h be piecewise polynomial approximations of degree $m-1$ of z and v that are obtained by applying the iterated collocation method described in the Appendix to (6a) and (6b) respectively. Apply backward differentiation of \tilde{v}_h and \tilde{w}_h at $x = 1$ using $p \geq m+1$ nodal points x_i (see Appendix for their definition) to generate approximations of $v'(1)$ and $w'(1)$ that we write as $(\nabla_{p,h}\tilde{v}_h)(1)$ and $(\nabla_{p,h}\tilde{w}_h)'(1)$.*

Assume that $m-1 \geq \min\{1, K\beta\}$ and set

$$\tilde{c}_{1,h} = \frac{\gamma - \alpha\tilde{w}_h(1) - \beta(\nabla_{p,h}\tilde{w}_h)(1)}{\alpha\tilde{v}_h(1) + \beta(\nabla_{p,h}\tilde{z}_h)(1)} \quad (30)$$

and

$$\tilde{u}_h(x) = \tilde{c}_{1,h}\tilde{v}_h(x) - \tilde{w}_h(x) \quad \text{for } x \in (0, 1]. \quad (31)$$

Then for h sufficiently small, the quantity $\tilde{c}_{1,h}$ is well defined by (30) and

$$\|u - \tilde{u}_h\| \leq C \left[\beta \left(Kh^{m-1} + h^{m-\delta} \right) + Kh^m + h^{m+1-\delta} \right] \quad (32)$$

for some constant C , where the quantity K is defined in (44).

Proof By (48) one has

$$\|v - \tilde{v}_h\| + \|w - \tilde{w}_h\| \leq C \left(Kh^m + h^{m+1-\delta} \right).$$

The coarseness and smoothness of the mesh near $x = 1$ then implies that

$$|v'(1) - (\nabla_{p,h}\tilde{v}_h)'(1)| + |w'(1) - (\nabla_{p,h}\tilde{w}_h)'(1)| \leq C \left(Kh^{m-1} + h^{m-\delta} \right).$$

Consequently $\alpha\tilde{v}_h(1) + \beta(\nabla_{p,h}\tilde{v}_h)'(1) \neq 0$ for h sufficiently small by Lemmas 2 and 3. It follows that the approximation (30) of (10) satisfies

$$|c_1 - \tilde{c}_{1,h}| \leq C \left[\beta \left(Kh^{m-1} + h^{m-\delta} \right) + Kh^m + h^{m+1-\delta} \right] \quad (33)$$

and furthermore the approximation $\tilde{u}_h(x)$ satisfies (32). \square

Remark 5 [Method I versus Method II] The error bound for Method II that is proved in Theorem 5 is inferior to the error bound in Theorem 4 for Method I except when one has a Dirichlet boundary condition at $x = 1$ in (3); on the other hand, Method II is simpler to implement. Thus when one has a Dirichlet condition at $x = 1$, Method II is to be preferred. Furthermore, our numerical experience with various boundary conditions at $x = 1$ shows that in practice the bound in (32) is always $O(Kh^m + h^{m+1-\delta})$ for $m - 1 \geq 0$, so Method II is in general competitive with Method I. This improvement of (32) will be investigated elsewhere.

4 Numerical results

To check the sharpness of the theoretical convergence bounds in Theorems 4 and 5, we test Methods I and II (where weighted product quadrature as described in (37) is used in both methods) on a single problem of the form (3) for the cases of Dirichlet and Neumann boundary conditions at $x = 1$. In each numerical example one has

$$u(x) = (0.3)^{-1} [E_{1-\delta,1}(0.3x^{1-\delta}) - 1] + 2x^{2-\delta} - x^{3-2\delta} - 3x^3 + 0.5x^4,$$

$$b(x) = 1 - 0.7 \cos(2.3x^2 - x^3) \quad \text{and} \quad c(x) \equiv 0,$$

with $(\alpha, \beta) = (1, 0)$ or $(0, 1)$. The Mittag-Leffler function E used here was defined in (7). The function f on the right-hand side of (3a) is specified by $Lu = f$ and γ is chosen such that (3b) is satisfied

Our example is constructed to have a known solution u that mimics as far as possible the behaviour of a typical solution of (3). For one can easily check that the derivatives of our u behave exactly as predicted by (17); furthermore, $b(x) = 0.3 + O(x^2)$ near $x = 0$ and the function $\phi(x) := (0.3)^{-1}[E_{1-\delta, 1}(0.3x^{1-\delta}) - 1]$ is a solution of $-D^{2-\delta}\phi + 0.3\phi' = 0$, as can be seen using $D^{2-\delta} = DD^{1-\delta}$ and [3, Theorem 4.3], so u has a singular component that near $x = 0$ lies (almost exactly) in the null space of the differential operator as required by Remark 2.

Example 3 Neumann condition at $x = 1$, Method I.

Results are presented in Tables 1–6; each table is for particular choices of m and the collocation parameters $\{c_1, c_2, \dots, c_m\}$ in our collocation method. The convergence rates obtained agree exactly with Theorem 4.

Table 1 Method I, case $\alpha = 0, \beta = 1$: $\max |(u - u_h)(x_i)|$ for $m = 1, c_k = \{0\}$; $K \neq 0$.

	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$	$N = 2^{13}$
$\delta = 0.1$	1.92e-2 1.01	9.58e-3 1.00	4.78e-3 1.00	2.39e-3 1.00	1.19e-3 1.00	5.97e-4 1.00	2.98e-4
$\delta = 0.3$	2.92e-2 1.01	1.45e-2 1.00	7.23e-3 1.00	3.61e-3 1.00	1.80e-3 1.00	9.00e-4 1.00	4.50e-4
$\delta = 0.5$	5.30e-2 1.02	2.61e-2 1.02	1.29e-2 1.01	6.39e-3 1.01	3.18e-3 1.01	1.58e-3 1.00	7.89e-4
$\delta = 0.7$	1.29e-1 1.04	6.28e-2 1.04	3.06e-2 1.03	1.50e-2 1.03	7.34e-3 1.02	3.61e-3 1.02	1.78e-3
$\delta = 0.9$	6.29e-1 1.02	3.10e-1 1.02	1.53e-1 1.02	7.56e-2 1.02	3.72e-2 1.03	1.83e-2 1.03	8.97e-3

Table 2 Method I, case $\alpha = 0, \beta = 1$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 1, c_k = \{\frac{1}{2}\}; K = 0$.

	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$	$N = 2^{13}$
$\delta = 0.1$	7.50e-5 1.82	2.12e-5 1.83	5.98e-6 1.84	1.68e-6 1.84	4.67e-7 1.85	1.30e-7 1.85	3.59e-8
$\delta = 0.3$	5.49e-4 1.63	1.77e-4 1.65	5.64e-5 1.66	1.79e-5 1.67	5.62e-6 1.67	1.76e-6 1.68	5.49e-7
$\delta = 0.5$	3.03e-3 1.45	1.11e-3 1.47	4.00e-4 1.48	1.44e-4 1.48	5.14e-5 1.49	1.83e-5 1.49	6.51e-6
$\delta = 0.7$	1.52e-2 1.26	6.31e-3 1.28	2.61e-3 1.28	1.07e-3 1.29	4.37e-4 1.29	1.78e-4 1.30	7.26e-5
$\delta = 0.9$	9.52e-2 1.12	4.37e-2 1.11	2.03e-2 1.10	9.47e-3 1.10	4.43e-3 1.10	2.07e-3 1.10	9.66e-4

Table 3 Method I, case $\alpha = 0, \beta = 1$: $\max |(u - u_h)(x_i)|$ for $m = 2, c_k = \{0, 1\}; K \neq 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$
$\delta = 0.1$	8.33e-4 2.00	2.08e-4 2.00	5.21e-5 2.00	1.30e-5 2.00	3.26e-6 2.00	8.14e-7 2.00	2.04e-7
$\delta = 0.3$	9.96e-4 1.99	2.50e-4 2.00	6.26e-5 2.00	1.57e-5 2.00	3.92e-6 2.00	9.81e-7 2.00	2.45e-7
$\delta = 0.5$	1.09e-3 1.98	2.78e-4 1.98	7.02e-5 1.99	1.77e-5 1.99	4.44e-6 2.00	1.11e-6 2.00	2.79e-7
$\delta = 0.7$	1.82e-3 1.98	4.62e-4 1.98	1.17e-4 1.98	2.97e-5 1.98	7.50e-6 1.99	1.89e-6 1.99	4.76e-7
$\delta = 0.9$	2.20e-2 1.93	5.75e-3 1.92	1.52e-3 1.93	3.99e-4 1.93	1.04e-4 1.94	2.72e-5 1.95	7.06e-6

Table 4 Method I, case $\alpha = 0, \beta = 1$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 2, c_k = \{0, \frac{2}{3}\};$ $K = 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$
$\delta = 0.1$	6.41e-6 2.86	8.80e-7 2.87	1.21e-7 2.87	1.65e-8 2.88	2.24e-9 2.88	3.05e-10 2.88	4.14e-11
$\delta = 0.3$	3.41e-5 2.64	5.47e-6 2.66	8.67e-7 2.67	1.36e-7 2.68	2.13e-8 2.68	3.32e-9 2.69	5.15e-10
$\delta = 0.5$	1.11e-4 2.42	2.08e-5 2.44	3.83e-6 2.46	6.96e-7 2.47	1.25e-7 2.48	2.24e-8 2.49	4.00e-9
$\delta = 0.7$	2.11e-4 2.68	3.30e-5 2.63	5.34e-6 2.55	9.11e-7 2.48	1.64e-7 2.41	3.08e-8 2.37	5.97e-9
$\delta = 0.9$	1.25e-2 2.14	2.83e-3 2.06	6.77e-4 2.04	1.65e-4 2.04	4.01e-5 2.05	9.72e-6 2.05	2.34e-6

Example 4 Neumann condition at $x = 1$, Method II.

Results are presented in Tables 7–10. This is the sole example where our numerical results are better than the rates predicted by our theory: while (32) guarantees

Table 5 Method I, case $\alpha = 0$, $\beta = 1$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 3$, $c_k = \{0, \frac{1}{3}, 1\}$; $K \neq 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$
$\delta = 0.1$	2.09e-6 3.00	2.61e-7 3.00	3.25e-8 3.00	4.06e-9 3.00	5.08e-10 3.00	6.35e-11
$\delta = 0.3$	2.37e-6 3.01	2.94e-7 3.01	3.67e-8 3.00	4.57e-9 3.00	5.70e-10 3.00	7.11e-11
$\delta = 0.5$	1.42e-5 2.98	1.80e-6 2.99	2.27e-7 2.99	2.86e-8 3.00	3.58e-9 3.00	4.48e-10
$\delta = 0.7$	9.11e-5 2.94	1.18e-5 2.94	1.54e-6 2.95	2.00e-7 2.96	2.56e-8 2.97	3.26e-9
$\delta = 0.9$	1.63e-3 2.86	2.25e-4 2.94	2.93e-5 2.91	3.90e-6 2.90	5.24e-7 2.91	6.99e-8

Table 6 Method I, case $\alpha = 0$, $\beta = 1$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 3$, $c_k = \{0, \frac{1}{2}, 1\}$; $K = 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$
$\delta = 0.1$	2.24e-7 3.93	1.46e-8 3.96	9.41e-10 3.97	6.00e-11 3.98	3.80e-12 3.97	2.42e-13
$\delta = 0.3$	8.47e-7 3.77	6.21e-8 3.79	4.49e-9 3.79	3.23e-10 3.79	2.34e-11 3.78	1.71e-12
$\delta = 0.5$	4.53e-6 3.49	4.02e-7 3.52	3.50e-8 3.53	3.04e-9 3.52	2.64e-10 3.52	2.30e-11
$\delta = 0.7$	3.23e-5 3.23	3.45e-6 3.28	3.54e-7 3.31	3.57e-8 3.32	3.58e-9 3.32	3.59e-10
$\delta = 0.9$	7.00e-4 2.93	9.20e-5 3.07	1.10e-5 3.13	1.25e-6 3.16	1.40e-7 3.17	1.56e-8

only $O(Kh^{m-1} + h^{m-\delta})$, the actual rates observed are $O(h^m)$ when $K \neq 0$ and $O(h^{m+1-\delta})$ when $K = 0$.

Example 5 Dirichlet condition at $x = 1$, Method II.

When one has a Dirichlet boundary condition at $x = 1$, Method II has the same convergence bound as Method I and is moreover simpler to implement, so we do not consider Method I for this example. Tables 11–16 present the errors and rates of convergence for Method II. The convergence rates in these tables match exactly the rates predicted by Theorem 5.

Table 7 Method II, case $\alpha = 0, \beta = 1$: $\max |(u - u_h)(x_i)|$ for $m = 1, c_k = \{0\}$, 3-point backward differencing using $\{x_{N-2}, x_{N-1}, x_N\}$ (NOTE: 2-point backward differencing produces similar rates of convergence, but somewhat larger errors); $K \neq 0$.

	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$	$N = 2^{13}$
$\delta = 0.1$	2.57e-2 1.01	1.28e-2 1.00	6.39e-3 1.00	3.19e-3 1.00	1.60e-3 1.00	7.98e-4 1.00	3.99e-4 1.00
$\delta = 0.3$	4.06e-2 1.01	2.01e-2 1.01	1.00e-2 1.00	4.99e-3 1.00	2.49e-3 1.00	1.25e-3 1.00	6.22e-4 1.00
$\delta = 0.5$	7.48e-2 1.03	3.66e-2 1.02	1.80e-2 1.02	8.91e-3 1.01	4.42e-3 1.01	2.20e-3 1.01	1.09e-3 1.01
$\delta = 0.7$	1.85e-1 1.05	8.94e-2 1.05	4.32e-2 1.04	2.10e-2 1.04	1.03e-2 1.03	5.02e-3 1.03	2.47e-3 1.02
$\delta = 0.9$	9.18e-1 1.02	4.54e-1 1.01	2.25e-1 1.02	1.11e-1 1.02	5.46e-2 1.03	2.68e-2 1.03	1.31e-2 1.03

Table 8 Method II, case $\alpha = 0, \beta = 1$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 1, c_k = \{\frac{1}{2}\}$, 3-point backward differencing using $\{x_{N-2}, x_{N-1}, x_N\}$; $K = 0$.

	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$	$N = 2^{13}$
$\delta = 0.1$	3.06e-4 1.95	7.93e-5 1.95	2.06e-5 1.94	5.35e-6 1.94	1.39e-6 1.94	3.62e-7 1.94	9.45e-8 1.94
$\delta = 0.3$	1.09e-3 1.73	3.29e-4 1.73	9.94e-5 1.72	3.01e-5 1.72	9.13e-6 1.72	2.78e-6 1.71	8.47e-7 1.71
$\delta = 0.5$	5.17e-3 1.50	1.83e-3 1.50	6.49e-4 1.50	2.29e-4 1.50	8.11e-5 1.50	2.87e-5 1.50	1.01e-5 1.50
$\delta = 0.7$	2.46e-2 1.28	1.01e-2 1.29	4.15e-3 1.29	1.69e-3 1.30	6.91e-4 1.30	2.81e-4 1.30	1.14e-4 1.30
$\delta = 0.9$	1.51e-1 1.16	6.74e-2 1.11	3.12e-2 1.10	1.45e-2 1.10	6.80e-3 1.10	3.18e-3 1.10	1.48e-3 1.10

5 Conclusions

It was shown that a two-point boundary value problem whose highest-order derivative is a Riemann-Liouville fraction derivative (of order $2 - \delta$, with $0 < \delta < 1$) could be reformulated in terms of a pair of weakly singular Volterra integral equations of the second kind. This reformulation enabled us to prove existence and uniqueness of a solution to the boundary value problem. It also led to the development of two efficient collocation methods for solving the original problem. One of these (Method II) is simpler than the other (Method I) but our error estimate

Table 9 Method II, case $\alpha = 0, \beta = 1$: $\max |(u - u_h)(x_i)|$ for $m = 2, c_k = \{0, 1\}$, 4-point backward differencing using $\{x_{N-3}, x_{N-2}, x_{N-1}, x_N\}$; $K \neq 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$
$\delta = 0.1$	2.22e-4 1.67	6.97e-5 1.84	1.94e-5 1.92	5.14e-6 1.96	1.32e-6 1.98	3.35e-7 1.99	8.43e-8
$\delta = 0.3$	5.80e-4 1.65	1.84e-4 1.83	5.18e-5 1.91	1.37e-5 1.96	3.54e-6 1.98	8.99e-7 1.99	2.27e-7
$\delta = 0.5$	1.61e-3 1.57	5.42e-4 1.79	1.57e-4 1.89	4.23e-5 1.94	1.10e-5 1.97	2.83e-6 1.98	7.16e-7
$\delta = 0.7$	4.23e-3 1.30	1.72e-3 1.65	5.47e-4 1.80	1.57e-4 1.88	4.26e-5 1.92	1.12e-5 1.95	2.90e-6
$\delta = 0.9$	1.17e-1 3.39	1.12e-2 2.45	2.05e-3 1.39	7.82e-4 1.64	2.51e-4 1.75	7.45e-5 1.83	2.10e-5

Table 10 Method II, case $\alpha = 0, \beta = 1$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 2, c_k = \{0, \frac{2}{3}\}$, 4-point backward differencing using $\{x_{N-3}, x_{N-2}, x_{N-1}, x_N\}$; $K = 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$
$\delta = 0.1$	2.50e-4 2.99	3.15e-5 2.99	3.96e-6 2.99	4.97e-7 2.99	6.24e-8 2.99	7.85e-9 2.99	9.88e-10
$\delta = 0.3$	6.88e-4 2.93	9.03e-5 2.93	1.18e-5 2.93	1.55e-6 2.92	2.05e-7 2.91	2.74e-8 2.89	3.68e-9
$\delta = 0.5$	2.59e-3 2.77	3.79e-4 2.76	5.60e-5 2.73	8.46e-6 2.69	1.31e-6 2.65	2.09e-7 2.62	3.39e-8
$\delta = 0.7$	1.38e-2 2.55	2.36e-3 2.51	4.16e-4 2.45	7.62e-5 2.39	1.45e-5 2.35	2.84e-6 2.32	5.67e-7
$\delta = 0.9$	2.32e-1 2.53	4.01e-2 2.42	7.48e-3 2.30	1.52e-3 2.21	3.29e-4 2.14	7.48e-5 2.10	1.75e-5

Table 11 Method II, case $\alpha = 1, \beta = 0$: $\max |(u - u_h)(x_i)|$ for $m = 1, c_k = \{0\}$; $K \neq 0$.

	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$	$N = 2^{13}$
$\delta = 0.1$	1.00e-2 1.00	5.02e-3 1.00	2.51e-3 1.00	1.26e-3 1.00	6.28e-4 1.00	3.14e-4 1.00	1.57e-4
$\delta = 0.3$	1.53e-2 1.01	7.63e-3 1.00	3.80e-3 1.00	1.90e-3 1.00	9.48e-4 1.00	4.74e-4 1.00	2.37e-4
$\delta = 0.5$	2.80e-2 1.02	1.38e-2 1.02	6.80e-3 1.02	3.36e-3 1.01	1.67e-3 1.01	8.29e-4 1.01	4.13e-4
$\delta = 0.7$	7.12e-2 1.03	3.49e-2 1.04	1.70e-2 1.04	8.29e-3 1.03	4.05e-3 1.03	1.98e-3 1.03	9.75e-4
$\delta = 0.9$	3.47e-1 0.89	1.88e-1 0.94	9.76e-2 0.98	4.94e-2 1.01	2.46e-2 1.0	1.21e-2 1.03	5.96e-3

for Method II is, for certain data, less good than our error estimate for Method I.

Nevertheless, our numerical experience has been that both methods achieve the

Table 12 Method II, case $\alpha = 1, \beta = 0$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 1, c_k = \{\frac{1}{2}\}$; $K = 0$.

	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$	$N = 2^{13}$
$\delta = 0.1$	2.33e-4 1.89	6.26e-5 1.90	1.68e-5 1.90	4.51e-6 1.90	1.21e-6 1.90	3.24e-7 1.90	8.68e-8
$\delta = 0.3$	1.14e-3 1.69	3.53e-4 1.70	1.09e-4 1.70	3.36e-5 1.70	1.03e-5 1.70	3.18e-6 1.70	9.80e-7
$\delta = 0.5$	5.35e-3 1.48	1.91e-3 1.49	6.79e-4 1.50	2.41e-4 1.50	8.53e-5 1.50	3.02e-5 1.50	1.07e-5
$\delta = 0.7$	2.55e-2 1.27	1.06e-2 1.29	4.33e-3 1.29	1.77e-3 1.30	7.21e-4 1.30	2.93e-4 1.30	1.19e-4
$\delta = 0.9$	1.70e-1 1.04	8.27e-2 1.07	3.95e-2 1.08	1.87e-2 1.09	8.77e-3 1.09	4.11e-3 1.10	1.92e-3

Table 13 Method II, case $\alpha = 1, \beta = 0$: $\max |(u - u_h)(x_i)|$ for $m = 2, c_k = \{0, 1\}$; $K \neq 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$
$\delta = 0.1$	1.82e-4 2.00	4.54e-5 2.00	1.13e-5 2.00	2.84e-6 2.00	7.09e-7 2.00	1.77e-7 2.00	4.43e-8
$\delta = 0.3$	4.42e-4 1.99	1.11e-4 2.00	2.79e-5 2.00	6.98e-6 2.00	1.75e-6 2.00	4.37e-7 2.00	1.09e-7
$\delta = 0.5$	1.24e-3 1.96	3.17e-4 1.97	8.07e-5 1.98	2.04e-5 1.99	5.15e-6 1.99	1.30e-6 1.99	3.25e-7
$\delta = 0.7$	4.17e-3 1.89	1.13e-3 1.91	2.99e-4 1.93	7.82e-5 1.95	2.03e-5 1.96	5.21e-6 1.97	1.33e-6
$\delta = 0.9$	2.07e-2 1.68	6.44e-3 1.76	1.90e-3 1.81	5.43e-4 1.84	1.51e-4 1.87	4.14e-5 1.89	1.12e-5

Table 14 Method II, case $\alpha = 1, \beta = 0$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 2, c_k = \{0, \frac{2}{3}\}$; $K = 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$	$N = 2^{12}$
$\delta = 0.1$	2.14e-5 2.88	2.91e-6 2.89	3.92e-7 2.90	5.27e-8 2.90	7.07e-9 2.90	9.48e-10 2.90	1.27e-10
$\delta = 0.3$	1.30e-4 2.66	2.05e-5 2.68	3.21e-6 2.69	4.98e-7 2.69	7.69e-8 2.70	1.19e-8 2.70	1.83e-9
$\delta = 0.5$	8.08e-4 2.43	1.50e-4 2.46	2.73e-5 2.47	4.92e-6 2.48	8.79e-7 2.49	1.57e-7 2.49	2.78e-8
$\delta = 0.7$	5.68e-3 2.18	1.25e-3 2.23	2.68e-4 2.25	5.62e-5 2.27	1.17e-5 2.28	2.41e-6 2.28	4.97e-7
$\delta = 0.9$	8.38e-2 1.86	2.30e-2 1.96	5.92e-3 2.01	1.47e-3 2.04	3.56e-4 2.06	8.53e-5 2.07	2.03e-5

same rates of convergence in practice; a theoretical justification of this observation is a topic for future research.

Table 15 Method II, case $\alpha = 1, \beta = 0$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 3, c_k = \{0, \frac{1}{3}, 1\}$; $K \neq 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$
$\delta = 0.1$	1.14e-6 3.04	1.39e-7 3.02	1.71e-8 3.01	2.11e-9 3.01	2.63e-10 3.00	3.28e-11
$\delta = 0.3$	2.66e-6 3.06	3.19e-7 3.04	3.89e-8 3.02	4.78e-9 3.02	5.90e-10 3.01	7.32e-11
$\delta = 0.5$	5.59e-6 3.03	6.82e-7 3.01	8.45e-8 3.01	1.05e-8 3.01	1.30e-9 3.01	1.62e-10
$\delta = 0.7$	1.38e-5 3.15	1.56e-6 3.05	1.88e-7 3.01	2.32e-8 3.00	2.91e-9 2.99	3.65e-10
$\delta = 0.9$	1.37e-3 2.84	1.91e-4 3.06	2.28e-5 3.14	2.60e-6 3.16	2.91e-7 3.11	3.38e-8

Table 16 Method II, case $\alpha = 1, \beta = 0$: $\max |(u - u_h)(x_i + c_k h_i)|$ for $m = 3, c_k = \{0, \frac{1}{2}, 1\}$; $K = 0$.

	$N = 2^6$	$N = 2^7$	$N = 2^8$	$N = 2^9$	$N = 2^{10}$	$N = 2^{11}$
$\delta = 0.1$	3.16e-7 3.84	2.21e-8 3.87	1.51e-9 3.89	1.02e-10 3.89	6.87e-12 3.90	4.59e-13
$\delta = 0.3$	1.33e-6 3.61	1.08e-7 3.66	8.59e-9 3.68	6.70e-10 3.69	5.19e-11 3.70	4.01e-12
$\delta = 0.5$	3.93e-6 3.33	3.90e-7 3.42	3.63e-8 3.47	3.28e-9 3.49	2.93e-10 3.50	2.60e-11
$\delta = 0.7$	1.16e-5 3.50	1.03e-6 3.44	9.45e-8 3.42	8.86e-9 3.38	8.48e-10 3.36	8.26e-11
$\delta = 0.9$	1.21e-3 2.79	1.75e-4 3.01	2.17e-5 3.10	2.53e-6 3.14	2.86e-7 3.15	3.22e-8

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A The piecewise polynomial collocation method

In this appendix we describe briefly the collocation method of [1,6,7] that is used to solve Volterra integral equations of the form

$$W(x) - J^{1-\delta}(bW)(x) - J^{1-\delta} \left((b' + c) \int_0^{(\cdot)} W \right) (x) = J^{1-\delta} g(x) \quad \text{for } x \in [0, 1] \quad (34)$$

where $g \in C^{q,\delta}(0, 1]$ is arbitrary.

Let N be a positive integer. Divide $[0, 1]$ by the mesh $0 = x_0 < x_1 < \dots < x_N = 1$, where $x_i = (i/N)^\rho$ for $i = 0, 1, \dots, N$. The user-chosen parameter $\rho \in [1, \infty)$ determines the grading of the mesh; when $\rho = 1$ the mesh is uniform.

Set $h_i = x_{i+1} - x_i$ for $i = 1, 2, \dots, N$. Set $h = \max h_i$.

Let m be a user-chosen positive integer. When solving (34) numerically, our computed solution W_h will lie in the space

$$S_{m-1}^{-1} := \left\{ v : v|_{(x_i, x_{i+1})} \in \pi_{m-1}, i = 0, 1, \dots, N-1 \right\} \quad (35)$$

comprising piecewise polynomials of degree at most $m-1$ that may be discontinuous at interior mesh points x_i . The set of collocation points in each mesh interval $[x_i, x_{i+1}]$ is

$$X_h := \{x_i + c_j h_i : 0 \leq c_1 < c_2 < \dots < c_m \leq 1, i = 0, 1, \dots, N-1\} \quad (36)$$

where the collocation parameters $\{c_j\}$ are chosen by the user. If $c_1 = 0$ and $c_m = 1$, then ϕ_h will lie in the space $S_{m-1}^{-1} \cap C[0, 1] =: S_{m-1}^0$, and (to make the number of equations equal to the number of unknowns) we require W_h to satisfy the initial condition $W_h(0) = 0$ when solving (34) because $W(0) = 0$.

As in [6], let $P_N : C[0, 1] \rightarrow S_{m-1}^{-1}$ be the piecewise polynomial of degree at most $m-1$ that interpolates at each collocation point in X_h . Then the *collocation solution* $W_h \in S_{m-1}^{-1}$ of (34) is defined, for all $x \in X_h \cup \{1\}$, by

$$W_h(x) - J^{1-\delta} P_N(bW_h)(x) - J^{1-\delta} P_N \left((b' + c) \int_{t=0}^{\cdot} W_h \right) (x) = J^{1-\delta} P_N g(x). \quad (37)$$

Here *weighted product quadrature*, with the collocation points as nodes, has been used to evaluate each integral $J^{1-\delta}(\cdot)$. That is, on each mesh interval $[x_{i-1}, x_i]$ the function $(\phi, \text{ say})$ that multiplies $(x-t)^{-\delta}$ in each expression $J^{1-\delta}(\dots)(x)$ is replaced by the polynomial $P_N \phi$ of degree $m-1$ that interpolates to ϕ at the collocation points $x_{i-1} + c_j h_i$, $j = 1, 2, \dots, m$, then the resulting integrals are evaluated exactly; this procedure is described fully in [1, §6.2.2].

Imitating [2,6], we shall assume here that all integrals are evaluated exactly. That is, instead of (37) we consider

$$W_h(x) - J^{1-\delta}(bW_h)(x) - J^{1-\delta} \left((b' + c) \int_{t=0}^{\cdot} W_h \right) (x) = J^{1-\delta} g(x) \text{ for all } x \in X_h \cup \{1\}. \quad (38)$$

The extension of our analysis to take weighted product quadrature into account will be considered in a separate paper. Note that in [7] we dealt with weighted product quadrature for a similar method, but the data b, c, g lay in the smoother space $C^q[0, 1]$.

In the analysis that follows, since the formulas become complicated, for convenience we omit the $(b' + c) \int W_h$ term from (38); relative to bW_h it is a lower-order term that will not influence materially any of our results.

We must show first that W_h is well defined by (38) for all sufficiently large N . Define $B : L_\infty[0, 1] \rightarrow L_\infty[0, 1]$ by $(B\phi)(x) := b(x)\phi(x)$ for $x \in [0, 1]$. Then (38) is equivalent to

$$W_h - P_N J^{1-\delta} B W_h = P_N J^{1-\delta} g \quad (39)$$

(note that $P_N W_h = W_h$). Let \mathcal{L} denote the space of all bounded linear operators from $(C^{q,\delta}(0, 1], \|\cdot\|_\infty)$ to itself. From [2, Lemma 2.2] and $\|B\|_{\mathcal{L}} \leq \|b\|_\infty$ it follows that $J^{1-\delta} B : (C^{q,\delta}(0, 1], \|\cdot\|_\infty) \rightarrow (C^{q,\delta}(0, 1], \|\cdot\|_\infty)$ is compact. The compactness of $J^{1-\delta} B$ and the Fredholm alternative imply that $(I - J^{1-\delta} B)^{-1}$ exists and is in \mathcal{L} . But $\|J^{1-\delta} B - P_N J^{1-\delta} B\|_{\mathcal{L}} \rightarrow 0$ as $N \rightarrow \infty$ by a minor variation of [2, Lemma 3.2]. Hence $(I - P_N J^{1-\delta} P_N B)^{-1}$ exists and is in \mathcal{L} — i.e., W_h is well defined by (39) — for all sufficiently large N .

Next, from (34) and (39) it follows that

$$W_h - W = (I - P_N J^{1-\delta} B)^{-1} (P_N - I) J^{1-\delta} (g + BW). \quad (40)$$

From above we have $\|(I - P_N J^{1-\delta} P_N B)^{-1}\|_{\mathcal{L}} \leq C$. We know that $g \in C^{q,\delta}(0, 1]$. Also, $BW \in C^{q,\delta}(0, 1]$ by [2, Lemma 2.1] and $J^{1-\delta}$ maps $C^{q,\delta}(0, 1]$ to itself [2, Lemma 2.2]. Thus

$$\|(P_N - I) J^{1-\delta} (g + BW)\|_\infty \leq Ch^m \quad \text{for } \rho \geq m/(1 - \delta) \quad (41)$$

by [6, (5.21)] (discarding a factor $\ln N$ in the case $\rho = m/(1 - \delta)$). Consequently (40) yields

$$\|W - W_h\|_\infty \leq Ch^m \quad \text{for } \rho \geq m/(1 - \delta), \quad (42)$$

provided N is sufficiently large.

Next, we prove that by a judicious choice of the collocation points one can ensure superconvergence of the computed solution W_h at these points. By the definition of P_N one has $P_N W = W$ at each collocation point. Now

$$(I - P_N J^{1-\delta} B)(P_N W - W_h) = P_N (J^{1-\delta} B W + J^{1-\delta} g) - P_N J^{1-\delta} B P_N W - P_N J^{1-\delta} g,$$

from (34) and (39). Thus

$$P_N W - W_h = (I - P_N J^{1-\delta} B)^{-1} P_N J^{1-\delta} (B W - B P_N W).$$

Here we know that $\|(I - P_N J^{1-\delta} P_N B)^{-1}\|_{\mathcal{L}} \leq C$ for N sufficiently large and $\|P_N\|_{\mathcal{L}} \leq C$ by [2, (3.16)], so

$$\|P_N W - W_h\|_{\infty} \leq C \|J^{1-\delta} B (I - P_N) W\|_{\infty}. \quad (43)$$

Set

$$K = \left| \int_0^1 \prod_{j=1}^m (s - c_j) ds \right|. \quad (44)$$

Then there exists a constant C (depending on V) such that for $\rho \geq m/(1 - \delta)$ one has

$$\|J^{1-\delta} B (I - P_N) W\|_{\infty} \leq C (K h^m + h^{m+1-\delta}); \quad (45)$$

for the case $K \neq 0$ in (45), simply invoke [6, (5.21)], while if $K = 0$, on taking $n = 1, \mu = 1, \nu = \delta$ and $s = 0$ in the argument in [10, pp.128–131], by inspection one sees that this calculation extends to our situation with singularities at the diagonal $y = x$ and the boundary $y = 0$, and one obtains (45) with $K = 0$. Therefore (43) yields

$$\|P_N W - W_h\|_{\infty} \leq C (K h^m + h^{m+1-\delta}) \quad \text{for } \rho \geq m/(1 - \delta) \text{ and } N \text{ sufficiently large,} \quad (46)$$

i.e., one has superconvergence of the computed solution W_h at the collocation points when $K = 0$.

The *iterated collocation solution* W_h^{it} is then defined [1, Section 6.2.1] by

$$W_h^{it}(x) = J^{1-\delta} (b W_h)(x) + J^{1-\delta} \left((b' + c) \int_0^{(\cdot)} W_h \right) (x) + J^{1-\delta} g(x) \quad (47)$$

for $x \in [0, 1]$. Note that $W_h^{it}(x) = W_h(x)$ for $x \in X_h \cup \{1\}$.

By subtracting (47) from (34) we get

$$W - W_h^{it} = J^{1-\delta} B (W - W_h) = J^{1-\delta} B (I - P_N) W + J^{1-\delta} B (P_N W - W_h).$$

Hence

$$\|W - W_h^{it}\|_{\infty} \leq C (K h^m + h^{m+1-\delta}) \quad \text{for } \rho \geq m/(1 - \delta) \text{ and } N \text{ sufficiently large,} \quad (48)$$

by (45) and (46).

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