Journal of
Mechanics of
Materials and Structures

VARIATIONAL METHODS FOR THE SOLUTION OF FRACTIONAL DISCRETE/CONTINUOUS STURM–LIOUVILLE PROBLEMS

Ricardo Almeida, Agnieszka B. Malinowska, M. Luísa Morgado and Tatiana Odzijewicz

Volume 12, No. 1 January 2017

msp

JOURNAL OF MECHANICS OF MATERIALS AND STRUCTURES
Vol. 12, No. 1, 2017
dx.doi.org/10.2140/jomms.2017.12.3

VARIATIONAL METHODS FOR THE SOLUTION OF FRACTIONAL DISCRETE/CONTINUOUS STURM–LIOUVILLE PROBLEMS

RICARDO ALMEIDA, AGNIESZKA B. MALINOWSKA,
M. LUÍSA MORGADO AND TATIANA ODZIJEWICZ

The fractional Sturm–Liouville eigenvalue problem appears in many situations, e.g., while solving anomalous diffusion equations coming from physical and engineering applications. Therefore, obtaining solutions or approximations of solutions to this problem is of great importance. Here, we describe how the fractional Sturm–Liouville eigenvalue problem can be formulated as a constrained fractional variational principle and show how such formulation can be used in order to approximate the solutions. Numerical examples are given to illustrate the method.

1. Introduction

Fractional calculus is a mathematical approach dealing with integral and differential terms of noninteger order. The concept of fractional calculus appeared shortly after calculus itself, but the development of practical applications proceeded very slowly. Only during the last few decades, fractional problems have increasingly attracted the attention of many researchers. Applications of fractional operators include chaotic dynamics [Zaslavsky 2005], material sciences [Mainardi 2010], mechanics of fractal and complex media [Carpinteri and Mainardi 1997; Li and Ostoja-Starzewski 2011], quantum mechanics [Hilfer 2000], physical kinetics [Zaslavsky and Edelman 2004] and many others (see, e.g., [Domek and Pworak 2016; Tarasov 2010]). Fractional derivatives are nonlocal operators and therefore successfully applied in the study of nonlocal or time-dependent processes [Podlubny 1999]. The well-established application of fractional calculus in physics is in the framework of anomalous diffusion behavior [Blaszczyk and Ciesielski 2014; Chen et al. 2012; D'Ovidio 2012; Leonenko et al. 2013; Meerschaert 2012; Metzler and Klafter 2000]: large jumps in space are modeled by space-fractional derivatives of order between 1 and 2, while long waiting times are modeled by the time derivatives of order between 0 and 1. These partial fractional differential equations can be solved by the method of separating variables, which leads to the Sturm–Liouville and the Cauchy equations. It means that, if we are able to solve the fractional Sturm–Liouville problem and the Cauchy problem, then we can find a solution to the fractional diffusion equation. In this paper, we consider two basic approaches to the fractional Sturm–Liouville problem: discrete and continuous. In both cases, we note that the problem can be formulated as a constrained fractional variational principle. A fractional variational problem consists of finding the extremizer of a functional that depends on fractional derivatives (differences) subject to boundary conditions and possibly some extra constraints. It is worth pointing out that the fractional calculus of variations has itself remarkable applications in classical mechanics. Riewe [1996; 1997] showed that a Lagrangian involving

Keywords: fractional Sturm–Liouville problem, fractional calculus of variations, discrete fractional calculus, continuous fractional calculus.

fractional time derivatives leads to an equation of motion with nonconservative forces such as friction. For more about the fractional calculus of variations, we refer the reader to [Almeida et al. 2015; Klimek 2009; Malinowska and Torres 2012; Malinowska et al. 2015] while for various approaches to fractional Sturm–Liouville problems we refer to [Al-Mdallal 2009; 2010; Klimek et al. 2014; Klimek 2015; 2016; Zayernouri and Karniadakis 2013].

The paper is divided into two main parts dedicated to discrete (Section 2) and continuous (Section 3) fractional problems. In the first part, we give a constructive proof of the existence of orthogonal solutions to the discrete fractional Sturm–Liouville eigenvalue problem (Theorem 2.4) and show that the smallest and largest eigenvalues can be characterized as the optimal values of certain functionals (Theorems 2.5 and 2.7). Our results are illustrated by an example. In the second part, we recall the fractional variational principle and the spectral theorem for the continuous fractional Sturm–Liouville problem. Since for most problems involving fractional derivatives (equations or variational problems) one cannot provide methods to compute the exact solutions analytically, numerical methods should be used for solving such problems. Discretizing both the fractional Sturm–Liouville equation and the related isoperimetric variational problem, we show, by an example, how the variational method can be used for solving the fractional Sturm–Liouville problem.

2. Discrete fractional calculus

In this section, we explain a relationship between the fractional Sturm–Liouville difference problem and a constrained discrete fractional variational principle. Namely, it is possible to look for solutions of Sturm–Liouville fractional difference equations by solving finite-dimensional constrained optimization problems. We shall start with necessary preliminaries. There are various versions of fractional differences; we mention here those of [Díaz and Osler 1974; Miller and Ross 1989; Atıcı and Eloe 2009a; 2009b] and the Caputo difference [Abdeljawad 2011]. In this paper, we use the notion of Grünwald and Letnikov [Kaczorek 2011; Podlubny 1999].

Let us define the mesh points $x_j = a + jh$, $j = 0, 1, \dots, N$, where h denotes the uniform space step, and set $D = \{x_0, \dots, x_N\}$. In what follows, $\alpha \in \mathbb{R}$ and $0 < \alpha \leq 1$. Moreover, we set

$$a_i^{(\alpha)} := \begin{cases} 1 & \text{if } i = 0, \\ (-1)^i(\alpha(\alpha-1)\cdots(\alpha-i+1))/i! & \text{if } i = 1, 2, \dots. \end{cases} \tag{2-1}$$

Definition 2.1. The backward fractional difference of order α, where $0 < \alpha \leq 1$, of function $f : D \to \mathbb{R}$ is defined by

$$ {}_0\Delta_k^\alpha f(x_k) := \frac{1}{h^\alpha} \sum_{i=0}^{k} (-1)^i \frac{\alpha(\alpha-1)\cdots(\alpha-i+1)}{i!} f(x_{k-i}) \tag{2-2}$$

while

$$ {}_k\Delta_N^\alpha f(x_k) := \frac{1}{h^\alpha} \sum_{i=0}^{N-k} (-1)^i \frac{\alpha(\alpha-1)\cdots(\alpha-i+1)}{i!} f(x_{k+i}) \tag{2-3}$$

is the forward fractional difference of function f.

Fractional backward and forward differences are linear operators.

Theorem 2.2 [Ostalczyk 2008]. *Let f and g be two real functions defined on D and $\beta, \gamma \in \mathbb{R}$. Then*

$$\begin{aligned}
{}_0\Delta_k^\alpha[\gamma f(x_k) + \beta g(x_k)] &= \gamma\, {}_0\Delta_k^\alpha\, f(x_k) + \beta\, {}_0\Delta_k^\alpha\, g(x_k),\\
{}_k\Delta_N^\alpha[\gamma f(x_k) + \beta g(x_k)] &= \gamma\, {}_k\Delta_N^\alpha\, f(x_k) + \beta\, {}_k\Delta_N^\alpha\, g(x_k)
\end{aligned}$$

for all k.

The following formula for summation by parts for fractional operators will be essential for proving results concerning variational problems.

Lemma 2.3 [Bourdin et al. 2013]. *Let f and g be two real functions defined on D. Then*

$$\sum_{k=0}^{N} g(x_k)\, {}_0\Delta_k^\alpha\, f(x_k) = \sum_{k=0}^{N} f(x_k)\, {}_k\Delta_N^\alpha\, g(x_k).$$

If $f(x_0) = f(x_N) = 0$ or $g(x_0) = g(x_N) = 0$, then

$$\sum_{k=1}^{N} g(x_k)\, {}_0\Delta_k^\alpha\, f(x_k) = \sum_{k=0}^{N-1} f(x_k)\, {}_k\Delta_N^\alpha\, g(x_k). \tag{2-4}$$

2A. *The Sturm–Liouville problem.* The topic of this subsection is the Sturm–Liouville fractional difference equation

$${}_k\Delta_N^\alpha(p(x_k)\, {}_0\Delta_k^\alpha\, y(x_k)) + q(x_k)y(x_k) = \lambda r(x_k)y(x_k), \quad k = 1, \dots, N-1, \tag{2-5}$$

with boundary conditions

$$y(x_0) = 0, \quad y(x_N) = 0. \tag{2-6}$$

We assume that $p(x_i) > 0$, $r(x_i) > 0$, $q(x_i)$ is defined and real-valued for all x_i, $i = 0, \dots, N$, and λ is a parameter. It is required to find the eigenfunctions and the eigenvalues of the given boundary value problem, i.e., the nontrivial solutions of (2-5)–(2-6) and the corresponding values of the parameter λ. The theorem below gives an answer to this question.

Theorem 2.4. *The Sturm–Liouville problem* (2-5)–(2-6) *has $N-1$ real eigenvalues, which we denote by*

$$\lambda_1 \le \lambda_2 \le \dots \le \lambda_{N-1}.$$

The corresponding eigenfunctions,

$$y^1, y^2, \dots, y^{N-1} : \{x_1, \dots, x_{N-1}\} \to \mathbb{R},$$

are mutually orthogonal: if $i \neq j$, then

$$\langle y^i, y^j\rangle_r := \sum_{k=1}^{N-1} r(x_k) y^i(x_k) y^j(x_k) = 0.$$

Furthermore, they span $\mathbb{R}^{N-1}$: any vector $\varphi = (\varphi(x_k))_{k=1}^{N-1} \in \mathbb{R}^{N-1}$ has a unique expansion

$$\varphi(x_k) = \sum_{i=1}^{N-1} c_i y^i(x_k), \quad 1 \le k \le N-1.$$

The coefficients c_i are given by

$$c_i = \frac{\langle \varphi, y^i \rangle_r}{\langle y^i, y^i \rangle_r}.$$

Proof. Observe that equations (2-5)–(2-6) can be considered as a system of $N-1$ linear equations with $N-1$ real unknowns $y(x_1), \ldots, y(x_{N-1})$. The corresponding matrix form is

$$Ay^T = \lambda R y^T, \tag{2-7}$$

where the entries A_{ij} of A are

$$A_{ij}^{(\alpha)} = \begin{cases} (1/h^{2\alpha})\big[q(x_i) + \sum_{k=0}^{N-i} (a_k^{(\alpha)})^2 p(x_{i+k})\big] & \text{if } i = j, \\ (1/h^{2\alpha})\big[\sum_{k=0}^{N-i} a_k^{(\alpha)} p(x_{i+k}) \sum_{m=0}^{k+i} a_m^{(\alpha)}\big] \text{ and } k-m+i = j & \text{if } i \neq j \end{cases}$$

and $R = \operatorname{diag}\{r(x_1), \ldots, r(x_{N-1})\}$. Writing (2-7) as

$$R^{-1} A y^T = \lambda y^T, \tag{2-8}$$

we get an eigenvalue problem with the symmetric matrix $R^{-1}A$. Because of the equivalence of problem (2-5)–(2-6) to problem (2-8), it follows from matrix theory that the Sturm–Liouville problem (2-5)–(2-6) has $N-1$ linearly pairwise orthogonal real independent eigenfunctions with all eigenvalues real. Now we would like to find constants $c_1, \ldots, c_{N-1}$ such that $\varphi(x_k) = \sum_{i=1}^{N-1} c_i y^i(x_k)$, $1 \le k \le N-1$. Note that

$$\langle \varphi, y^j \rangle_r = \left\langle \sum_{i=1}^{N-1} c_i y^i, y^j \right\rangle_r = \sum_{i=1}^{N-1} c_i \langle y^i, y^j \rangle_r = c_j \langle y^j, y^j \rangle_r$$

because of orthogonality. Therefore, $c_i = \langle \varphi, y^i \rangle_r / \langle y^i, y^i \rangle_r$, $1 \le i \le N-1$. □

2B. *Isoperimetric variational problems.* In this section, we prove two theorems connecting the Sturm–Liouville problem (2-5)–(2-6) to isoperimetric problems of discrete fractional calculus of variations.

Theorem 2.5. *Let y^1 denote the first eigenfunction, normalized to satisfy the isoperimetric constraint*

$$I[y] = \sum_{k=1}^{N} r(x_k)(y(x_k))^2 = 1 \tag{2-9}$$

associated with the first eigenvalue λ_1 of problem (2-5)–(2-6). *Then y^1 is a minimizer of functional*

$$J[y] = \sum_{k=1}^{N} \big[p(x_k)({}_0\Delta_k^\alpha y(x_k))^2 + q(x_k)(y(x_k))^2\big] \tag{2-10}$$

subject to boundary conditions $y(x_0) = 0$ and $y(x_N) = 0$ and isoperimetric constraint (2-9). *Moreover, $J[y^1] = \lambda_1$.*

Proof. Suppose that y is a minimizer of J. Then by [Malinowska and Odzijewicz 2016, Theorem 5], there exists a real constant λ such that y satisfies

$${}_k\Delta_N^\alpha(p(x_k)\, {}_0\Delta_k^\alpha y(x_k)) + q(x_k)y(x_k) - \lambda r(x_k)y(x_k) = 0, \quad k = 1, \ldots, N-1, \tag{2-11}$$

together with $y(x_0)=0$ and $y(x_N)=0$ and isoperimetric constraint (2-9). Let us multiply (2-11) by $y(x_k)$ and sum up from $k=1$ to $N-1$; then

$$\sum_{k=1}^{N-1}\left[y(x_k)\,{}_k\Delta_N^{\alpha}(p(x_k)\,{}_0\Delta_k^{\alpha}\,y(x_k))+q(x_k)(y(x_k))^2\right]=\sum_{k=1}^{N-1}\lambda r(x_k)(y(x_k))^2.$$

By summation by parts (2-4),

$$\sum_{k=1}^{N-1}y(x_k)\,{}_k\Delta_N^{\alpha}(p(x_k)\,{}_0\Delta_k^{\alpha}\,y(x_k))=\sum_{k=1}^{N}p(x_k)({}_0\Delta_k^{\alpha}\,y(x_k))^2.$$

As (2-9) holds and $y(x_N)=0$, we obtain

$$J[y]=\lambda.$$

Any solution to problem (2-9)–(2-10) that satisfies (2-11) must be nontrivial since (2-9) holds, so λ must be an eigenvalue. According to Theorem 2.4, eigenvalue λ_1 is the smallest element of the spectrum and has corresponding eigenfunction $y^{(1)}$ normalized to meet the isoperimetric condition. Therefore, $J[y^{(1)}]=\lambda_1$. □

Definition 2.6. We will call functional R defined by

$$R[y]=\frac{J[y]}{I[y]},$$

where $J[y]$ is given by (2-10) and $I[y]$ by (2-9), the Rayleigh quotient for the fractional discrete Sturm–Liouville problem (2-5)–(2-6).

Theorem 2.7. *Assume that y satisfies boundary conditions $y(x_0)=y(x_N)=0$ and is nontrivial.*

(i) *If y is a minimizer of Rayleigh quotient R for the Sturm–Liouville problem* (2-5)–(2-6), *then the value of R in y is equal to the smallest eigenvalue λ_1, i.e.*, $R[y]=\lambda_1$.

(ii) *If y is a maximizer of Rayleigh quotient R for the Sturm–Liouville problem* (2-5)–(2-6), *then the value of R in y is equal to the largest eigenvalue λ_{N-1}, i.e.*, $R[y]=\lambda_{N-1}$.

Proof. We give the proof only for (i) as the second case can be proved similarly. Suppose that y satisfying boundary conditions $y(x_0)=y(x_N)=0$ and being nontrivial is a minimizer of Rayleigh quotient R and that value of R in y is equal to λ. Consider the functions

$$\begin{aligned}&\phi:[-\varepsilon,\varepsilon]\to\mathbb{R},\\&\qquad h\mapsto I[y+h\eta]=\sum_{k=1}^{N}r(x_k)(y(x_k)+h\eta(x_k))^2,\\&\psi:[-\varepsilon,\varepsilon]\to\mathbb{R},\\&\qquad h\mapsto J[y+h\eta]=\sum_{k=1}^{N}\left[p(x_k)({}_0\Delta_k^{\alpha}(y(x_k)+h\eta(x_k)))^2+q(x_k)(y(x_k)+h\eta(x_k))^2\right],\\&\zeta:[-\varepsilon,\varepsilon]\to\mathbb{R},\\&\qquad h\mapsto R[y+h\eta]=\frac{J[y+h\eta]}{I[y+h\eta]},\end{aligned}$$

where $\eta : D \to \mathbb{R}$ with $\eta(x_0) = \eta(x_N) = 0$ and $\eta \neq 0$. Since ζ is of class C^1 on $[-\varepsilon, \varepsilon]$ and

$$\zeta(0) \leq \zeta(h), \quad |h| \leq \varepsilon,$$

we deduce that

$$\zeta'(0) = \frac{d}{dh} R[y + h\eta]\Big|_{h=0} = 0.$$

Moreover, notice that

$$\zeta'(h) = \frac{1}{\phi(h)}\left(\psi'(h) - \frac{\psi(h)}{\phi(h)}\phi'(h)\right)$$

and

$$\psi'(0) = \frac{d}{dh} J[y + h\eta]\Big|_{h=0} = 2\sum_{k=1}^{N}\big[p(x_k)\, {}_0\Delta_k^\alpha\, y(x_k)\, {}_0\Delta_k^\alpha\, \eta(x_k) + q(x_k)y(x_k)\eta(x_k)\big],$$

$$\phi'(0) = \frac{d}{dh} I[y + h\eta]\Big|_{h=0} = 2\sum_{k=1}^{N} r(x_k)y(x_k)\eta(x_k).$$

Therefore,

$$\begin{aligned}
\zeta'(0) &= \frac{d}{dh} R[y + h\eta]\Big|_{h=0} \\
&= \frac{2}{I[y]}\left[\sum_{k=1}^{N}\big[p(x_k)\, {}_0\Delta_k^\alpha\, y(x_k)\, {}_0\Delta_k^\alpha\, \eta(x_k) + q(x_k)y(x_k)\eta(x_k)\big] - \frac{J[y]}{I[y]}\sum_{k=1}^{N} r(x_k)y(x_k)\eta(x_k)\right] = 0.
\end{aligned}$$

Having in mind that $J[y]/I[y] = \lambda$ and $\eta(x_0) = \eta(x_N) = 0$ and using summation by parts (2-4), we obtain

$$\sum_{k=1}^{N-1}\big[{}_k\Delta_N^\alpha(p(x_k)\, {}_0\Delta_k^\alpha\, y(x_k)) + q(x_k)y(x_k) - \lambda r(x_k)y(x_k)\big]\eta(x_k) = 0.$$

Since η is arbitrary, we have

$${}_k\Delta_N^\alpha(p(x_k)\, {}_0\Delta_k^\alpha\, y(x_k)) + q(x_k)y(x_k) - \lambda r(x_k)y(x_k) = 0, \quad k = 1, \ldots, N-1. \tag{2-12}$$

As $y \neq 0$, we have that λ is an eigenvalue of (2-12). On the other hand, let λ_i be an eigenvalue and y^i the corresponding eigenfunction; then

$${}_k\Delta_N^\alpha(p(x_k)\, {}_0\Delta_k^\alpha\, y_i(x_k)) + q(x_k)y_i(x_k) = \lambda_i r(x_k)y^i(x_k). \tag{2-13}$$

Similarly to the proof of Theorem 2.5, we can obtain

$$\frac{\sum_{k=1}^{N}\big[p(x_k)({}_0\Delta_k^\alpha\, y^i(x_k))^2 + q(x_k)(y^i(x_k))^2\big]}{\sum_{k=1}^{N} r(x_k)(y^i(x_k))^2} = \lambda_i$$

for any $1 \leq i \leq N-1$. That is, $R[y^i] = J[y^i]/I[y^i] = \lambda_i$. Finally, since the minimum value of R at y is equal to λ, i.e.,

$$\lambda \leq R[y^i] = \lambda_i \quad \text{for all } i \in \{1, \ldots, N-1\},$$

we have $\lambda = \lambda_1$. □

α	λ_1	λ_2	λ_3
0.25	0.7102065750	1.148567387	1.349294886
0.50	0.6004483933	1.353660384	1.831047473
0.75	0.5779798778	1.632135974	2.496488153
1	0.5857864376	2.0	3.414213562

Table 1. Eigenvalues of (2-16) for different values of α.

Example 2.8. Let us consider the following problem: minimize

$$J[y] = \sum_{k=1}^{N} ({}_0\Delta_k^\alpha\, y(x_k))^2 \tag{2-14}$$

subject to

$$I[y] = \sum_{k=1}^{N} (y(x_k))^2 = 1 \tag{2-15}$$

and $y(x_0) = y(x_N) = 0$, where N is fixed. In this case, the Euler–Lagrange equation takes the form

$${}_k\Delta_N^\alpha\, {}_0\Delta_k^\alpha\, y(x_k) = \lambda y(x_k), \quad k = 1, \dots, N-1. \tag{2-16}$$

Together with boundary conditions $y(x_0) = y(x_N) = 0$, it is the Sturm–Liouville eigenvalue problem where $p(x_i) = 1$, $r(x_i) = 1$ and $q(x_i) = 0$ for $k = 1, \dots, N-1$. Let us choose $N = 4$ and $h = 1$. Eigenvalues of (2-16) for different values of α are presented in Table 1. Those results are obtained by solving the matrix eigenvalue problem of the form (2-8).

Observe that problem (2-14)–(2-15) can be treated as a finite-dimensional constrained optimization problem. Namely, the problem is to minimize function J of $N-1$ variables $y_1 = y(x_1), \dots, y_{N-1} = y(x_{N-1})$ on the $(N-1)$-dimensional sphere with equation $\sum_{k=1}^{N-1} y_k^2 = 1$. Table 2 and Figure 1 present the solution to problem (2-14)–(2-15) for $N = 4$, $h = 1$ and different values of α. By Theorem 2.5, the first eigenvalue λ_1 of (2-16) is the minimum value of J on $\sum_{k=1}^{N-1} y_k^2 = 1$ and the first eigenfunction of (2-16) is the minimizer of this problem. Other eigenfunctions and eigenvalues of (2-16) we can find by using the first-order necessary optimality conditions (Karush–Kuhn–Tucker conditions), that is, by solving the system of equations

$$\begin{cases} \dfrac{\partial J}{\partial y_k} = \lambda \dfrac{\partial I}{\partial y_k}, \\ \sum_{k=1}^{N-1} y_k^2 = 1, \end{cases} \qquad k = 1, \dots, N-1. \tag{2-17}$$

α	$y(x_1)$	$y(x_2)$	$y(x_3)$	λ_1
0.25	0.52042378274	0.65949734450	0.54242265711	0.7102065749
0.50	0.50954825567	0.67778735991	0.53006119446	0.6004483933
0.75	0.50509466979	0.69443334582	0.51248580736	0.5779798777
1	0.49999999999	0.70710678118	0.5	0.5857864376

Table 2. The solution to problem (2-14)–(2-15) for different values of α.

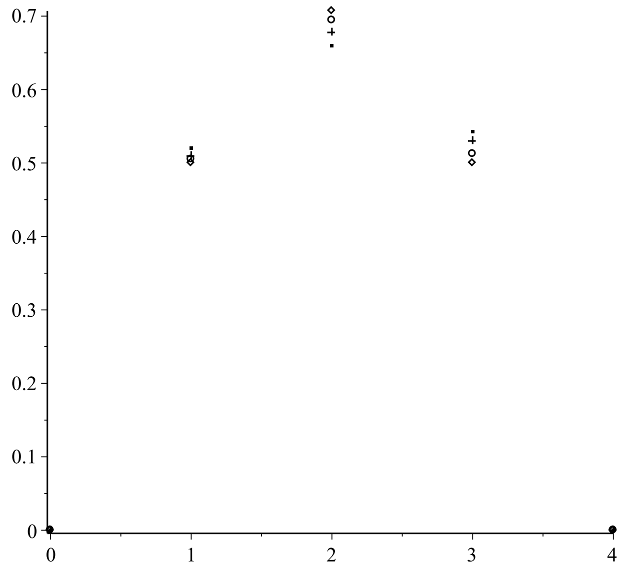

Figure 1. The solution to problem (2-14)–(2-15) for $\alpha = \frac{1}{4}$ $(\cdot)$, $\frac{1}{2}$ $(+)$, $\frac{3}{4}$ $(\circ)$ and 1 $(\diamond)$.

3. Continuous fractional calculus

This section is devoted to the continuous fractional Sturm–Liouville problem and its formulation as a constrained fractional variational principle. Namely, we shall show that this formulation can be used to approximate the solutions. As in the discrete case, there are several different definitions for fractional derivatives [Kilbas et al. 2006]; the most well-known are the Grünwald–Letnikov, the Riemann–Liouville and the Caputo fractional derivatives.

Definition 3.1. Let $f : [a, b] \to \mathbb{R}$ be a function and α a positive real number such that $0 < \alpha < 1$. We define the left and right Riemann–Liouville fractional derivatives of order α by

$$
\begin{aligned}
{}_aD_x^\alpha f(x) &:= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x (x-t)^{-\alpha} f(t)\, dt, \\
{}_xD_b^\alpha f(x) &:= \frac{-1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_x^b (t-x)^{-\alpha} f(t)\, dt
\end{aligned}
$$

and the left and right Caputo fractional derivatives of order α by

$$
\begin{aligned}
{}_a^CD_x^\alpha f(x) &:= \frac{1}{\Gamma(1-\alpha)} \int_a^x (x-t)^{-\alpha} f'(t)\, dt, \\
{}_x^CD_b^\alpha f(x) &:= \frac{-1}{\Gamma(1-\alpha)} \int_x^b (t-x)^{-\alpha} f'(t)\, dt.
\end{aligned}
$$

The Caputo derivative seems more suitable in applications. Let us recall that the Caputo derivative of a constant is zero, whereas the Riemann–Liouville is not. Moreover, the Laplace transform, which is used for solving fractional differential equations, of the Riemann–Liouville derivative contains the limit values of the Riemann–Liouville fractional derivatives (of order $\alpha - 1$) at the lower terminal $x = a$.

Mathematically such problems can be solved, but there is no physical interpretation for such conditions. On the other hand, the Laplace transform of the Caputo derivative imposes boundary conditions involving the value of the function at the lower point $x = a$, which usually are acceptable physical conditions.

The Grünwald–Letnikov definition is a generalization of the ordinary discretization formulas for integer-order derivatives.

Definition 3.2. Let $0 < \alpha < 1$ be real. The left and right Grünwald–Letnikov fractional derivatives of order α of a function f are defined as

$$
\begin{aligned}
{}^{\mathrm{GL}}_{a}D^{\alpha}_{x}\, f(x) &:= \lim_{h\to 0^+} \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} f(x-kh),\\
{}^{\mathrm{GL}}_{x}D^{\alpha}_{b}\, f(x) &:= \lim_{h\to 0^+} \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} f(x+kh).
\end{aligned}
$$

Here $\binom{\alpha}{k}$ stands for the generalization of binomial coefficients to real numbers (see (2-1)). However, in this section for historical reasons, we denote

$$
(w^{\alpha}_{k}) := (-1)^k \binom{\alpha}{k}
$$

rather than $a^{(\alpha)}_{i}$.

Relations between those three types of derivatives are given below.

Proposition 3.3 [Podlubny 1999]. *Let us assume the function f is integrable in $[a, b]$. Then the Riemann–Liouville fractional derivatives exist and coincide with Grünwald–Letnikov fractional derivatives.*

Proposition 3.4 [Kilbas et al. 2006]. *Let us assume that f is a function for which the Caputo fractional derivatives exist together with the Riemann–Liouville fractional derivatives in $[a, b]$. Then, if $0 < \alpha < 1$,*

$$
\begin{aligned}
{}^{C}_{a}D^{\alpha}_{x}\, f(x) &= {}_{a}D^{\alpha}_{x}\, f(x) - \frac{f(a)}{\Gamma(1-\alpha)}(x-a)^{-\alpha},\\
{}^{C}_{x}D^{\alpha}_{b}\, f(x) &= {}_{x}D^{\alpha}_{b}\, f(x) - \frac{f(b)}{\Gamma(1-\alpha)}(b-x)^{-\alpha}.
\end{aligned}
\tag{3-1}
$$

If $f(a) = 0$ or $f(b) = 0$, then ${}^{C}_{a}D^{\alpha}_{x}\, f(x) = {}_{a}D^{\alpha}_{x}\, f(x)$ or ${}^{C}_{x}D^{\alpha}_{b}\, f(x) = {}_{x}D^{\alpha}_{b}\, f(x)$, respectively.

It is well-known that we can approximate the Riemann–Liouville fractional derivative using the Grünwald–Letnikov fractional derivative. Given the interval $[a, b]$ and a partition of the interval $x_j = a + jh$, for $j = 0, 1, \dots, N$ and some $h > 0$ such that $x_N = b$, we have

$$
\begin{aligned}
{}_{a}D^{\alpha}_{x_j}\, f(x_j) &= \frac{1}{h^{\alpha}} \sum_{k=0}^{j} (w^{\alpha}_{k}) f(x_{j-k}) + O(h),\\
{}_{x_j}D^{\alpha}_{b}\, f(x_j) &= \frac{1}{h^{\alpha}} \sum_{k=0}^{N-j} (w^{\alpha}_{k}) f(x_{j+k}) + O(h);
\end{aligned}
$$

that is, the truncated Grünwald–Letnikov fractional derivatives are first-order approximations of the Riemann–Liouville fractional derivatives. Using relations (3-1), we deduce a decomposition sum for the Caputo fractional derivatives:

$$ {}_{a}^{C}D_{x_j}^{\alpha} f(x_j) \approx \frac{1}{h^\alpha}\sum_{k=0}^{j}(w_k^\alpha) f(x_{j-k}) - \frac{f(a)}{\Gamma(1-\alpha)}(x_j-a)^{-\alpha} =: {}_{a}^{C}\widetilde{D}_{x_j}^{\alpha} f(x_j), \tag{3-2} $$

$$ {}_{x_j}^{C}D_{b}^{\alpha} f(x_j) \approx \frac{1}{h^\alpha}\sum_{k=0}^{N-j}(w_k^\alpha) f(x_{j+k}) - \frac{f(b)}{\Gamma(1-\alpha)}(b-x_j)^{-\alpha} =: {}_{x_j}^{C}\widetilde{D}_{b}^{\alpha} f(x_j). \tag{3-3} $$

3A. ***Variational problem.*** Consider the following variational problem: minimize the functional

$$ I[y] = \int_a^b L(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x))\, dx, \tag{3-4} $$

subject to the boundary conditions

$$ y(a) = y_a, \quad y(b) = y_b, \quad y_a, y_b \in \mathbb{R}, \tag{3-5} $$

where $0 < \alpha < 1$ and the Lagrange function $L : [a, b] \times \mathbb{R}^2 \to \mathbb{R}$ is differentiable with respect to the second and third arguments.

Theorem 3.5 [Agrawal 2006]. *If $\bar{y}$ is a solution to* (3-4)–(3-5), *then $\bar{y}$ satisfies the fractional differential equation*

$$ \frac{\partial L}{\partial y}(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x)) + {}_{x}D_{b}^{\alpha} \frac{\partial L}{\partial\, {}_{a}^{C}D_{x}^{\alpha} y}(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x)) = 0, \quad t \in [a, b]. \tag{3-6} $$

Relations like (3-6) are known in the literature as the Euler–Lagrange equation and provide a necessary condition that every solution of the variational problem must satisfy. Adding to problem (3-4)–(3-5) an integral constraint

$$ \int_a^b g(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x))\, dx = K, \tag{3-7} $$

where K is a fixed constant and $g : [a, b] \times \mathbb{R}^2 \to \mathbb{R}$ is a differentiable function with respect to the second and third arguments, we get an isoperimetric variational problem. In order to obtain a necessary condition for a minimizer, we define the new function

$$ F := \lambda_0 L(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x)) - \lambda g(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x)), \tag{3-8} $$

where λ_0 and λ are Lagrange multipliers. Then every solution $\bar{y}$ of the fractional isoperimetric problem given by (3-4)–(3-5) and (3-7) is also a solution to the fractional differential equation [Almeida and Torres 2011]

$$ \frac{\partial F}{\partial y}(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x)) + {}_{x}D_{b}^{\alpha} \frac{\partial F}{\partial\, {}_{a}^{C}D_{x}^{\alpha} y}(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x)) = 0, \quad t \in [a, b]. \tag{3-9} $$

Moreover, if $\bar{y}$ is not a solution to

$$ \frac{\partial g}{\partial y}(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x)) + {}_{x}D_{b}^{\alpha} \frac{\partial g}{\partial\, {}_{a}^{C}D_{x}^{\alpha} y}(x, y(x), {}_{a}^{C}D_{x}^{\alpha} y(x)) = 0, \quad t \in [a, b], \tag{3-10} $$

then we can put $\lambda_0 = 1$ in (3-8).

Discretization Method 1. Using the approximation formula for the Caputo fractional derivative given by (3-2), we can discretize functional (3-4) in the following way. Let $N \in \mathbb{N}$, $h = (b-a)/N$ and the grid $x_j = a + jh$, $j = 0, 1, \ldots, N$. Then

$$\begin{aligned} I[y] &= \sum_{k=1}^{N} \int_{x_{k-1}}^{x_k} L(x, y(x), {}_a^C D_x^\alpha\, y(x))\, dx \\ &\approx \sum_{k=1}^{N} hL(x_k, y(x_k), {}_a^C D_{x_k}^\alpha\, y(x_k)) \\ &\approx \sum_{k=1}^{N} hL(x_k, y(x_k), {}_a^C \widetilde{D}_{x_k}^\alpha\, y(x_k)). \end{aligned} \tag{3-11}$$

This is the direct way to solve the problem, using discretization techniques.

Discretization Method 2. By the previous discussion, the initial problem of minimization of the functional (3-4), subject to boundary conditions (3-5), can be numerically replaced by the finite-dimensional optimization problem

$$\Phi(y_1, \ldots, y_{N-1}) := \sum_{k=1}^{N} hL(x_k, y(x_k), {}_a^C \widetilde{D}_{x_k}^\alpha\, y(x_k)) \to \min,$$

subject to

$$y_0 = y_a, \quad y_N = y_b,$$

where $y_k := y(x_k)$.

Using the first-order necessary optimality conditions given by the system of $N-1$ equations

$$\frac{\partial \Phi}{\partial y_j} = 0 \quad \text{for all } j = 1, \ldots, N-1,$$

we get

$$\frac{\partial L}{\partial y}(x_j, y(x_j), {}_a^C \widetilde{D}_{x_j}^\alpha\, y(x_j)) + \sum_{k=0}^{N-j} \frac{(w_k^\alpha)}{h^\alpha} \frac{\partial L}{\partial\, {}_a^C D_x^\alpha\, y}(x_{j+k}, y(x_{j+k}), {}_a^C \widetilde{D}_{x_{j+k}}^\alpha\, y(x_{j+k})) = 0 \tag{3-12}$$

with $j = 1, \ldots, N-1$. As $N \to \infty$, that is, as $h \to 0$, the solutions of system (3-12) converge to the solutions of the fractional Euler–Lagrange equation associated with the variational problem [Pooseh et al. 2013, Theorem 4.1]. The constrained variational problem given by (3-4)–(3-5) and (3-7) can be solved similarly. More precisely, in this case, we have to replace the Lagrange function L by the augmented function $F = \lambda_0 L - \lambda g$ and proceed with similar calculations.

3B. *Sturm–Liouville problem.*

Consider the fractional differential equation

$$\left[{}^C D_b^\alpha\, p(x)\, {}^C D_a^\alpha + q(x)\right] y(x) = \lambda r_\alpha(x) y(x), \tag{3-13}$$

subject to the boundary conditions

$$y(a) = y(b) = 0. \tag{3-14}$$

Equation (3-13) together with condition (3-14) is called the fractional Sturm–Liouville problem. As in the discrete case, it is required to find the eigenfunctions and the eigenvalues of the given boundary value problem, i.e., the nontrivial solutions of (3-13)–(3-14) and the corresponding values of the parameter λ.

In what follows, we assume:

Assumption A. Let $\frac{1}{2} < \alpha < 1$ and p, q and r_α be given functions such that $p \in C^1[a,b]$ and $p(x) > 0$ for all $x \in [a,b]$, $q, r_\alpha \in C[a,b]$, $r_\alpha(x) > 0$ for all $x \in [a,b]$ and $(\sqrt{r_\alpha})'$ is Hölderian, of order $\beta \le \alpha - \frac{1}{2}$, on $[a,b]$.

Theorem 3.6 [Klimek et al. 2014]. *Under Assumption A, the fractional Sturm–Liouville problem* (3-13)–(3-14) *has an infinite increasing sequence of eigenvalues* $\lambda_1, \lambda_2, \dots,$ *and to each eigenvalue* λ_k, *there is a corresponding continuous eigenfunction* y_k *that is unique up to a constant factor.*

The fractional Sturm–Liouville problem can be remodeled as a fractional isoperimetric variational problem.

Theorem 3.7 [Klimek et al. 2014]. *Let Assumption A hold and* y^1 *be the eigenfunction, normalized to satisfy the isoperimetric constraint*

$$I[y] = \int_a^b r_\alpha(x) y^2(x)\, dx = 1, \tag{3-15}$$

associated with the first eigenvalue λ_1 *of problem* (3-13)–(3-14), *and assume that function* $D_b^\alpha(p\, {}^C D_a^\alpha\, y^1)$ *is continuous. Then* y^1 *is a minimizer of the variational functional*

$$J[y] = \int_a^b \left[p(x)({}^C D_a^\alpha\, y(x))^2 + q(x) y^2(x) \right] dx, \tag{3-16}$$

in the class of $C[a,b]$ *functions with* ${}^C D_a^\alpha\, y$ *and* $D_b^\alpha(p\, {}^C D_a^\alpha\, y)$ *continuous in* $[a,b]$, *subject to the boundary conditions*

$$y(a) = y(b) = 0 \tag{3-17}$$

and isoperimetric constraint (3-15). *Moreover,*

$$J[y^1] = \lambda_1.$$

Discretization Method 3. Using the approximation formula for the Caputo fractional derivatives given by (3-2)–(3-3), we can discretize (3-13) in the following way. Let $N \in \mathbb{N}$, $h = (b-a)/N$ and the grid $x_j = a + jh$, $j = 0, 1, \dots, N$. Then at $x = x_i$, (3-13) may be discretized as

$$\frac{h^{-2\alpha}}{r_\alpha(x_i)} \sum_{k=0}^{N-i} (w_k^\alpha) p(x_{i+k}) \sum_{l=0}^{i+k} (w_l^\alpha) y_{i+k-l} + \frac{q(x_i)}{r_\alpha(x_i)} y_i = \lambda y_i, \quad i = 1, \dots, N-1,$$

which in matrix form may be written as

$$AY = \lambda Y, \tag{3-18}$$

N	5	10	15
λ_1	4.603751971	4.491185175	4.426964914

Table 3. Values of λ_1 for $N = 5$, 10, 15.

where $Y = [y_1, y_2, \dots, y_{N-1}]$, $y_i = y(x_i)$, and $A = (c_{ik})$, $i = 1, 2, \dots, N-1$, $k = 1, 2, \dots, N-1$, with

$$c_{ik} = \begin{cases} (h^{-2\alpha}/r_\alpha(x_i)) \sum_{j=0}^{N-i} (w_j^\alpha)^2 p(x_{j+i}) + q(x_i)/r_\alpha(x_i) & \text{if } i = k, \\ (h^{-2\alpha}/r_\alpha(x_i)) \sum_{j=0}^{N-i} (w_j^\alpha)(w_{j+i-k}^\alpha) p(x_{j+i}) & \text{if } i > k, \\ (h^{-2\alpha}/r_\alpha(x_i)) \sum_{j=k-i}^{N-i} (w_j^\alpha)(w_{j+i-k}^\alpha) p(x_{j+i}) & \text{if } i < k, \end{cases}$$

reducing in this way the Sturm–Liouville problem to an algebraic eigenvalue problem.

Example 3.8. Let us consider the following problem: minimize the functional

$$\int_0^1 ({}_0^C D_x^\alpha\, y(x))^2\, dx, \tag{3-19}$$

under the restrictions

$$\int_0^1 y^2(x)\, dx = 1, \quad y(0) = y(1) = 0, \tag{3-20}$$

where $\alpha = \frac{3}{4}$. Since $y(0) = 0$, we have ${}_0^C D_x^\alpha\, y(x) = {}_0 D_x^\alpha\, y(x)$. Using Method 1, we obtain a finite-dimensional constrained optimization problem

$$\sum_{k=1}^{N} N^{2\alpha-1} \left(\sum_{i=0}^{k} (w_i^\alpha) y_{k-i} \right)^2 \to \min, \tag{3-21}$$

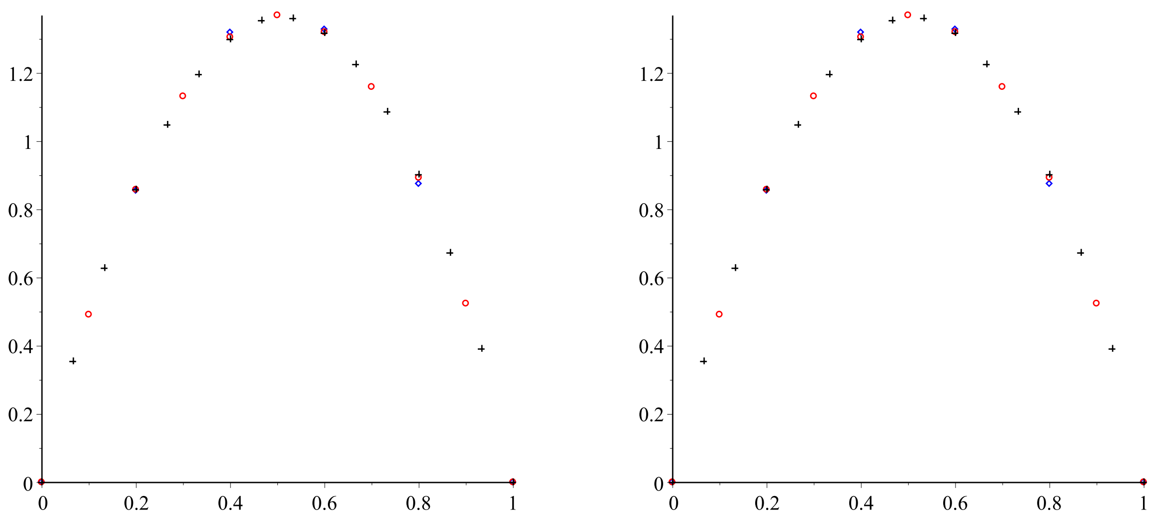

Figure 2. Approximations of solutions to problem (3-19)–(3-20) using Methods 1 (left) and 2 (right) with $N = 5$ ($\diamond$), 10 ($\circ$) and 15 ($+$).

N	5	10	15
λ_1	4.603751969	4.491185168	4.426964909
λ_2	13.67144835	14.31569449	14.33350940
λ_3	22.69092491	26.35335634	26.90113751
λ_4	29.24531071	39.48118456	41.37391615
λ_5		52.54234156	56.93534748
λ_6		64.64953668	73.03700902
λ_7		74.96494602	89.07875858
λ_8		82.83813371	104.5749014
λ_9		87.76536891	119.0339408
λ_{10}			132.0436041
λ_{11}			143.2212682
λ_{12}			152.2566950
λ_{13}			158.8942685
λ_{14}			162.9518168

Table 4. Values of λ_i for $N = 5, 10, 15$.

subject to

$$\sum_{k=1}^{N} \frac{y_k^2}{N} = 1, \quad y_0 = y_N = 0. \tag{3-22}$$

Using the Maple package Optimization, we get approximations of the optimal solutions to (3-19)–(3-20) for different values of N. Table 3 shows values of λ_1 for $N = 5, 10, 15$. Note that λ_1 is the value of (3-21), where $\bar{y} = [0, y_1, \ldots, y_{N-1}, 0]$ is the optimal solution to (3-21)–(3-22). In other words, λ_1 is an approximation of the minimum value of functional (3-19) and the first eigenvalue of the Sturm–Liouville problem (which is the Euler–Lagrange equation for the considered variational problem). Figure 2, left, presents minimizers $\bar{y}$ for $N = 5, 10, 15$.

Observe that the unique solution to the Euler–Lagrange equation (see (3-10)) associated with the integral constraint is $\bar{y}(x) = 0$. As $\bar{y}(x) = 0$ is not a solution to (3-19)–(3-20) (condition $\int_0^1 y^2(x)\,dx = 1$ fails), we can consider $\lambda_0 = 1$ in (3-8). Therefore, the auxiliary function is

$$F := ({}_0^C D_x^\alpha\, y(x))^2 - \lambda y^2(x).$$

Thus,

$$\Phi(y_1, \ldots, y_{N-1}) := \sum_{k=1}^{N} h(({}_0^C D_{x_k}^\alpha\, y_k)^2 - \lambda y_k^2),$$

and the computation of $\partial\Phi/\partial y_j$ leads to

$$-\lambda y_j + N^{2\alpha} \sum_{k=0}^{N-j} (w_k^\alpha) \sum_{l=0}^{j+k} (w_l^\alpha) y_{j+k-l} = 0, \quad j = 1, \ldots, N-1. \tag{3-23}$$

Solving system of equations (3-23) together with (3-22), we obtain not only an approximation of the optimal solution to problem (3-19)–(3-20) but also other solutions to the Euler–Lagrange equation (3-9)

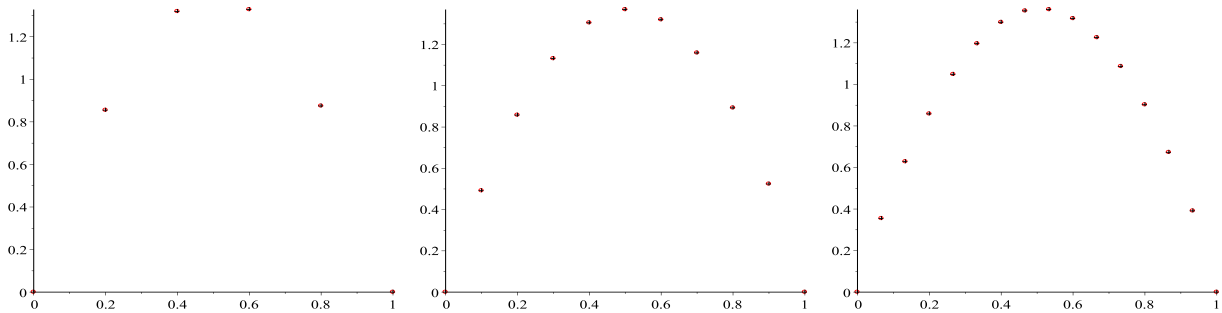

Figure 3. Approximations of solutions to problem (3-19)–(3-20) using Methods 1 (∘) and 2 (+) with $N = 5$ (left), 10 (center) and 15 (right).

as $N \to \infty$. In other words, we get some approximations of the eigenvalues and eigenfunctions of the Sturm–Liouville problem. Table 4 presents approximations of the eigenvalues obtained by this procedure for $N = 5$, 10, 15. In Figure 2, right, we present the eigenvectors, for $N = 5$, 10, 15, associated with the eigenvalues λ_1.

In Figure 3, we compare the approximation of the optimal solutions to (3-19)–(3-20), obtained by solving (3-21)–(3-22) (Method 1) and (3-23)–(3-22) (Method 2), for $N = 5$, 10, 15.

Now let us consider the Sturm–Liouville problem

$$^{C}D_1^{3/4}\, {}^{C}D_0^{3/4}\, y(x) = \lambda y(x), \tag{3-24}$$

subject to the boundary conditions

$$y(0) = y(1) = 0. \tag{3-25}$$

Under the conditions of Theorem 3.7, (3-24) is the Euler–Lagrange equation for isoperimetric problem

N	5	10	20	40	80	160
λ_1	4.603751972	4.491185175	4.387575384	4.314056432	4.264767769	4.231946921
λ_2	13.67144835	14.31569450	14.29943076	14.18275912	14.08194289	14.01015799
λ_3	22.69092491	26.35335634	27.02784640	27.01132309	26.88877847	26.78184511
λ_4	29.24531071	39.48118456	41.95747334	42.33045300	42.25841874	42.13429128
λ_5		52.54234157	58.40981791	59.60122278	59.68496380	59.56753673
λ_6		64.64953668	75.99486098	78.61012095	79.00578911	78.93437596
λ_7		74.96494602	94.25189512	99.05856280	99.96479334	99.98764503
λ_8		82.83813372	112.8375161	120.7904806	122.4632696	122.6454529
λ_9		87.76536891	131.3694072	143.5891552	146.3337902	146.7516690
λ_{10}			149.5318910	167.3194776	171.5033012	172.2513810
λ_{11}			166.9946039	191.8029693	197.8472756	199.0332700
λ_{12}			183.4744810	216.9142113	225.3053712	227.0563318
λ_{13}			198.6917619	242.4962397	253.7773704	256.2351380
λ_{14}			212.4063351	268.4292940	283.2100111	286.5368179

Table 5. Approximation of the eigenvalues using Method 3.

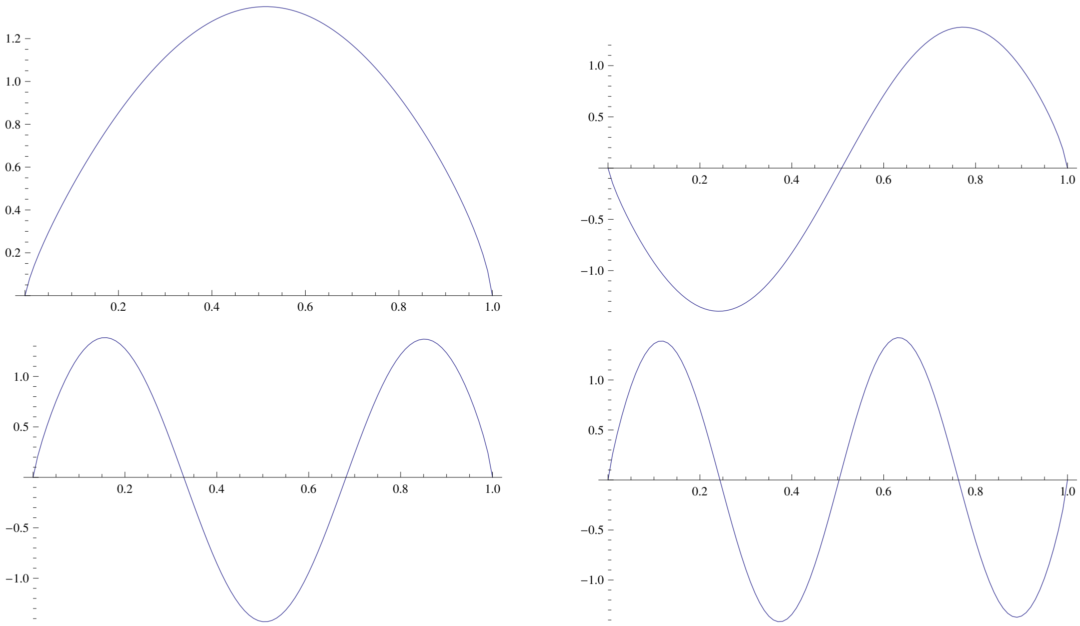

Figure 4. Normalized eigenfunctions obtained with $N = 100$, corresponding to the eigenvalues λ_1 (top left), λ_2 (top right), λ_3 (bottom left) and λ_4 (bottom right).

(3-19)–(3-20). Table 5 presents approximations of the eigenvalues of (3-24) obtained by Method 3 for $N = 5$, 10, 20, 40, 80, 160 (for $N = 20$, 40, 80, 160 only the first 14 eigenvalues are listed). Figure 4 shows normalized eigenfunctions, obtained for $N = 100$, corresponding to the eigenvalues λ_1, λ_2, λ_3, λ_4.

4. Conclusions

Since the seminal works [Nigmatullin 1986; Wyss 1986] were published, fractional differential equations have become a popular way to model anomalous diffusion. As stated in [Meerschaert 2012], this type of approach is the most reasonable: the fractional derivative in space represents large particle jumps (that lead to anomalous superdiffusion) while the time-fractional derivative models time delays between particle motion. Fractional diffusion equations have been used, e.g., to model pollution in ground water [Benson et al. 2001] and flow in porous media [He 1998]. Many other examples can be found in [Meerschaert 2012; Meerschaert and Sikorskii 2012].

It was proved in [Klimek et al. 2016] that, under appropriate assumptions, the space-time fractional diffusion equation

$$ {}^{C}D^{\beta}_{0+,t}\, u(t,x) = -\frac{1}{r_\alpha(x)}\big[{}^{C}D^{\alpha}_{b-,x}\, p(x)\, {}^{C}D^{\alpha}_{a+,x} + q(x)\big]u(t,x) \quad \text{for all } (t,x) \in (0,\infty)\times[a,b], \tag{4-1} $$

where $0 < \beta < 1$, $\frac{1}{2} < \alpha < 1$ and ${}^{C}D^{\beta}_{0+,t}$ and ${}^{C}D^{\alpha}_{b-,x}$, ${}^{C}D^{\alpha}_{a+,x}$ are partial fractional derivatives, with the boundary and initial conditions

$$ u(t,a) = u(t,b) = 0, \qquad t \in (0,\infty), \tag{4-2} $$

$$ u(0,x) = f(x), \qquad x \in [a,b], \tag{4-3} $$

has a continuous solution $u : [0, \infty) \times [a, b] \to \mathbb{R}$ given by the series

$$u(t, x) = \sum_{k=1}^{\infty} \langle y_k, f \rangle E_\beta(-\lambda_k t^\beta) y_k(x). \tag{4-4}$$

In (4-4), $\langle f, g \rangle := \int_a^b r_\alpha(x) f(x) g(x)\, dx$, E_β is the one-parameter Mittag–Leffler function and y_k and λ_k ($k = 1, 2, \dots$) are the eigenfunctions and the eigenvalues of the fractional Sturm–Liouville problem (3-13)–(3-14). Thus, numerical methods, presented in this paper, for finding the eigenvalues and eigenfunctions of fractional Sturm–Liouville problems can also be used to approximate solutions to fractional diffusion problems of the form (4-1)–(4-3). We have presented a link between fractional Sturm–Liouville and fractional isoperimetric variational problems that provides a possible method for solution of the former. Discrete problems with the Grünwald–Letnikov difference were analyzed: we proved the existence of orthogonal solutions to the discrete fractional Sturm–Liouville eigenvalue problem and showed that its eigenvalues can be characterized as values of certain functionals. For continuous problems with the Caputo fractional derivatives, in order to examine the performance of the proposed method, the approximation based on the shifted Grünwald–Letnikov definition was used. This type of discretization is most popular in practical applications, when numerically solving fractional diffusion equations, due to the fact that such methods are mass-preserving [Defterli et al. 2015].

Acknowledgements

Research was supported by Portuguese funds through the Center for Research and Development in Mathematics and Applications (CIDMA) and the Portuguese Foundation for Science and Technology (FCT) within UID/MAT/04106/2013 (Almeida) and UID/MAT/00013/2013 (Morgado), by the Bialystok University of Technology grant S/WI/1/2016 (Malinowska) and by the Warsaw School of Economics grant KAE/BMN16/18/16 (Odzijewicz).

References

[Abdeljawad 2011] T. Abdeljawad, "On Riemann and Caputo fractional differences", *Comput. Math. Appl.* **62**:3 (2011), 1602–1611.

[Agrawal 2006] O. P. Agrawal, "Fractional variational calculus and the transversality conditions", *J. Phys. A* **39**:33 (2006), 10375–10384.

[Al-Mdallal 2009] Q. M. Al-Mdallal, "An efficient method for solving fractional Sturm–Liouville problems", *Chaos Solitons Fractals* **40**:1 (2009), 183–189.

[Al-Mdallal 2010] Q. M. Al-Mdallal, "On the numerical solution of fractional Sturm–Liouville problems", *Int. J. Comput. Math.* **87**:12 (2010), 2837–2845.

[Almeida and Torres 2011] R. Almeida and D. F. M. Torres, "Necessary and sufficient conditions for the fractional calculus of variations with Caputo derivatives", *Commun. Nonlinear Sci. Numer. Simul.* **16**:3 (2011), 1490–1500.

[Almeida et al. 2015] R. Almeida, S. Pooseh, and D. F. M. Torres, *Computational methods in the fractional calculus of variations*, Imperial College, London, 2015.

[Atıcı and Eloe 2009a] F. M. Atıcı and P. W. Eloe, "Discrete fractional calculus with the nabla operator", *Electron. J. Qual. Theory Differ. Equ.* **Spec. Ed. I** (2009), 3.

[Atıcı and Eloe 2009b] F. M. Atıcı and P. W. Eloe, "Initial value problems in discrete fractional calculus", *Proc. Amer. Math. Soc.* **137**:3 (2009), 981–989.

[Benson et al. 2001] D. A. Benson, R. Schumer, M. M. Meerschaert, and S. W. Wheatcraft, "Fractional dispersion, Lévy motion, and the MADE tracer tests", *Transp. Porous Media* **42**:1–2 (2001), 211–240.

[Blaszczyk and Ciesielski 2014] T. Blaszczyk and M. Ciesielski, "Numerical solution of fractional Sturm–Liouville equation in integral form", *Fract. Calc. Appl. Anal.* **17**:2 (2014), 307–320.

[Bourdin et al. 2013] L. Bourdin, J. Cresson, I. Greff, and P. Inizan, "Variational integrator for fractional Euler–Lagrange equations", *Appl. Numer. Math.* **71** (2013), 14–23.

[Carpinteri and Mainardi 1997] A. Carpinteri and F. Mainardi (editors), *Fractals and fractional calculus in continuum mechanics* (Udine, Italy, 1996), CISM Courses and Lectures **378**, Springer, Vienna, 1997.

[Chen et al. 2012] Z.-Q. Chen, M. M. Meerschaert, and E. Nane, "Space-time fractional diffusion on bounded domains", *J. Math. Anal. Appl.* **393**:2 (2012), 479–488.

[Defterli et al. 2015] O. Defterli, M. D'Elia, Q. Du, M. Gunzburger, R. Lehoucq, and M. M. Meerschaert, "Fractional diffusion on bounded domains", *Fract. Calc. Appl. Anal.* **18**:2 (2015), 342–360.

[Díaz and Osler 1974] J. B. Díaz and T. J. Osler, "Differences of fractional order", *Math. Comp.* **28**:125 (1974), 185–202.

[Domek and Pworak 2016] S. Domek and P. Pworak (editors), *Theoretical developments and applications of non-integer order systems: 7th Conference on Non-Integer Order Calculus and Its Applications* (Szczecin, Poland, 2015), Lecture Notes in Electrical Engineering **357**, Springer, Cham, Switzerland, 2016.

[D'Ovidio 2012] M. D'Ovidio, "From Sturm–Liouville problems to fractional and anomalous diffusions", *Stochastic Process. Appl.* **122**:10 (2012), 3513–3544.

[He 1998] J.-H. He, "Approximate analytical solution for seepage flow with fractional derivatives in porous media", *Comput. Methods Appl. Mech. Engrg.* **167**:1–2 (1998), 57–68.

[Hilfer 2000] R. Hilfer (editor), *Applications of fractional calculus in physics*, World Scientific, River Edge, NJ, 2000.

[Kaczorek 2011] T. Kaczorek, *Selected problems of fractional systems theory*, Lecture Notes in Control and Information Sciences **411**, Springer, Berlin, 2011.

[Kilbas et al. 2006] A. A. Kilbas, H. M. Srivastava, and J. J. Trujillo, *Theory and applications of fractional differential equations*, North-Holland Mathematics Studies **204**, Elsevier, Amsterdam, 2006.

[Klimek 2009] M. Klimek, *On solutions of linear fractional differential equations of a variational type*, Monographs **172**, Czestochowa University of Technology, 2009.

[Klimek 2015] M. Klimek, "Fractional Sturm–Liouville problem and 1D space-time fractional diffusion with mixed boundary conditions", pp. 46808 in *Proceedings of the ASME 2015 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference* (Boston, 2015), vol. 9: 2015 ASME/IEEE International Conference on Mechatronic and Embedded Systems and Applications, American Society of Mechanical Engineers, New York, 2015.

[Klimek 2016] M. Klimek, "Fractional Sturm–Liouville problem in terms of Riesz derivatives", pp. 3–16 in *Theoretical developments and applications of non-integer order systems: 7th Conference on Non-Integer Order Calculus and Its Applications* (Szczecin, Poland, 2015), edited by S. Domek and P. Dworak, Lecture Notes in Electrical Engineering **357**, Springer, Cham, Switzerland, 2016.

[Klimek et al. 2014] M. Klimek, T. Odzijewicz, and A. B. Malinowska, "Variational methods for the fractional Sturm–Liouville problem", *J. Math. Anal. Appl.* **416**:1 (2014), 402–426.

[Klimek et al. 2016] M. Klimek, A. B. Malinowska, and T. Odzijewicz, "Applications of fractional Sturm–Liouville problem to the space-time fractional diffusion in a finite domain", *Fract. Calc. Appl. Anal.* **19**:2 (2016), 516–550.

[Leonenko et al. 2013] N. N. Leonenko, M. M. Meerschaert, and A. Sikorskii, "Fractional Pearson diffusions", *J. Math. Anal. Appl.* **403**:2 (2013), 532–546.

[Li and Ostoja-Starzewski 2011] J. Li and M. Ostoja-Starzewski, "Micropolar continuum mechanics of fractal media", *Internat. J. Engrg. Sci.* **49**:12 (2011), 1302–1310.

[Mainardi 2010] F. Mainardi, *Fractional calculus and waves in linear viscoelasticity: an introduction to mathematical models*, Imperial College, London, 2010.

[Malinowska and Odzijewicz 2016] A. B. Malinowska and T. Odzijewicz, "Multidimensional discrete-time fractional calculus of variations", pp. 17–28 in *Theoretical developments and applications of non-integer order systems: 7th Conference on Non-Integer Order Calculus and Its Applications* (Szczecin, Poland, 2015), edited by S. Domek and P. Dworak, Lecture Notes in Electrical Engineering **357**, Springer, Cham, Switzerland, 2016.

[Malinowska and Torres 2012] A. B. Malinowska and D. F. M. Torres, *Introduction to the fractional calculus of variations*, Imperial College, London, 2012.

[Malinowska et al. 2015] A. B. Malinowska, T. Odzijewicz, and D. F. M. Torres, *Advanced methods in the fractional calculus of variations*, Springer, Cham, Switzerland, 2015.

[Meerschaert 2012] M. M. Meerschaert, "Fractional calculus, anomalous diffusion, and probability", pp. 265–284 in *Fractional dynamics*, edited by J. Klafter et al., World Scientific, Hackensack, NJ, 2012.

[Meerschaert and Sikorskii 2012] M. M. Meerschaert and A. Sikorskii, *Stochastic models for fractional calculus*, Studies in Mathematics **43**, Walter de Gruyter, Berlin, 2012.

[Metzler and Klafter 2000] R. Metzler and J. Klafter, "The random walk's guide to anomalous diffusion: a fractional dynamics approach", *Phys. Rep.* **339**:1 (2000), 1–77.

[Miller and Ross 1989] K. S. Miller and B. Ross, "Fractional difference calculus", pp. 139–152 in *Univalent functions, fractional calculus, and their applications* (Kōriyama, Japan, 1988), edited by H. M. Srivastava and S. Owa, Horwood, Chichester, United Kingdom, 1989.

[Nigmatullin 1986] R. R. Nigmatullin, "The realization of the generalized transfer equation in a medium with fractal geometry", *Phys. Stat. Sol. B* **133**:1 (1986), 425–430.

[Ostalczyk 2008] P. Ostalczyk, *Zarys rachunku różniczkowo-całkowego ułamkowych rzedów: teoria i zastosowanie w automatyce*, Politechniki Łódzkiej, Łódż, Poland, 2008.

[Podlubny 1999] I. Podlubny, *Fractional differential equations: an introduction to fractional derivatives, fractional differential equations, to methods of their solution and some of their applications*, Mathematics in Science and Engineering **198**, Academic, San Diego, 1999.

[Pooseh et al. 2013] S. Pooseh, R. Almeida, and D. F. M. Torres, "Discrete direct methods in the fractional calculus of variations", *Comput. Math. Appl.* **66**:5 (2013), 668–676.

[Riewe 1996] F. Riewe, "Nonconservative Lagrangian and Hamiltonian mechanics", *Phys. Rev. E* (3) **53**:2 (1996), 1890–1899.

[Riewe 1997] F. Riewe, "Mechanics with fractional derivatives", *Phys. Rev. E* (3) **55**:3 (1997), 3581–3592.

[Tarasov 2010] V. E. Tarasov, *Fractional dynamics: applications of fractional calculus to dynamics of particles, fields and media*, Springer, Heidelberg, Germany, 2010.

[Wyss 1986] W. Wyss, "The fractional diffusion equation", *J. Math. Phys.* **27**:11 (1986), 2782–2785.

[Zaslavsky 2005] G. M. Zaslavsky, *Hamiltonian chaos and fractional dynamics*, Oxford University, 2005.

[Zaslavsky and Edelman 2004] G. M. Zaslavsky and M. A. Edelman, "Fractional kinetics: from pseudochaotic dynamics to Maxwell's Demon", *Phys. D* **193**:1–4 (2004), 128–147.

[Zayernouri and Karniadakis 2013] M. Zayernouri and G. E. Karniadakis, "Fractional Sturm–Liouville eigen-problems: theory and numerical approximation", *J. Comput. Phys.* **252** (2013), 495–517.

Received 30 Jan 2016. Revised 29 Mar 2016. Accepted 4 Apr 2016.

RICARDO ALMEIDA: ricardo.almeida@ua.pt
Center for Research and Development in Mathematics and Applications, Department of Mathematics, University of Aveiro, 3810-193 Aveiro, Portugal

AGNIESZKA B. MALINOWSKA: a.malinowska@pb.edu.pl
Faculty of Computer Science, Bialystok University of Technology, 15-351 Bialystok, Poland

M. LUÍSA MORGADO: luisam@utad.pt
Centro de Matemática, pólo CMAT-UTAD, Department of Mathematics, University of Trás-os-Montes e Alto Douro, 5000-801 Vila Real, Portugal

TATIANA ODZIJEWICZ: tatiana.odzijewicz@sgh.waw.pl
Department of Mathematics and Mathematical Economics, Warsaw School of Economics, 02-554 Warsaw, Poland

JOURNAL OF MECHANICS OF MATERIALS AND STRUCTURES

msp.org/jomms

Founded by Charles R. Steele and Marie-Louise Steele

Cover photo: Ev Shafrir

See msp.org/jomms for submission guidelines.

JoMMS (ISSN 1559-3959) at Mathematical Sciences Publishers, 798 Evans Hall #6840, c/o University of California, Berkeley, CA 94720-3840, is published in 10 issues a year. The subscription price for 2017 is US $615/year for the electronic version, and $775/year (+$60, if shipping outside the US) for print and electronic. Subscriptions, requests for back issues, and changes of address should be sent to MSP.

JoMMS peer-review and production is managed by EditFlow® from Mathematical Sciences Publishers.

PUBLISHED BY

mathematical sciences publishers

nonprofit scientific publishing

http://msp.org/

Journal of Mechanics of Materials and Structures

Volume 12, No. 1 January 2017

Special issue on
Coupled Field Problems and Multiphase Materials

1559-3959(2017)12:1;1-4