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

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Abstract. The fractional Sturm–Liouville eigenvalue problem appears in many situations, e.g., while solving anomalous diffusion equations coming from physical and engineering applications. Therefore to obtain solutions or approximation 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 non-integer order. The concept of fractional calculus appeared shortly after calculus itself, but the development of practical applications proceeded very slowly. Only during the last decades, fractional problems have increasingly attracted the attention of many researchers. Applications of fractional operators include chaotic dynamics [46], material sciences [29], mechanics of fractal and complex media [12, 28], quantum mechanics [19], physical kinetics [47] and many others (see e.g.,[15, 43]). Fractional derivatives are nonlocal operators and therefore successfully applied in the study of nonlocal or time-dependent processes [39]. The well-established application of fractional calculus in physics is in the framework of anomalous diffusion behavior [10, 13, 17, 27, 33, 35]: 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 in finding the extremizer of a functional that depends on fractional derivatives (differences) subject to boundary conditions and possibly some extra constraints. It is worthy to point out that the fractional calculus of variations has itself remarkable applications in classical mechanics. Riewe [41, 42] showed that a Lagrangian involving fractional time derivatives leads to an equation of motion with non-conservative forces such as friction. For more about the fractional calculus of variations we refer the reader to [6, 22, 30, 31] while for various approaches to fractional Sturm–Liouville problems we refer to [3, 4, 23, 24, 25, 45].

The paper is divided into two main parts dedicated, respectively, to discrete (Section 2) and continuous (Section 3) fractional problems. In the first part we give a constructive proof

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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 (Theorem 2.5 and Theorem 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 related with it 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 the fractional differences, we can mention here those introduced by Diaz and Osler [16], Miller and Ross [36], Atici and Eloe [7, 8] or the Caputo difference [1]. In this paper, we use the notion of Grünwald–Letnikov [20, 39].

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

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

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. *(cf. [38]) Let f, g be two real functions defined on D and $\beta, \gamma \in \mathbb{R}$. Then*

$$_0\Delta_k^\alpha[\gamma f(x_k) + \beta g(x_k)] = \gamma {_0\Delta_k^\alpha} f(x_k) + \beta {_0\Delta_k^\alpha} g(x_k),$$

$$_k\Delta_N^\alpha[\gamma f(x_k) + \beta g(x_k)] = \gamma {_k\Delta_N^\alpha} f(x_k) + \beta {_k\Delta_N^\alpha} g(x_k),$$

for all k.

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

Lemma 2.3. *(cf. [11]) Let f, 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.** In this subsection our topic is the Sturm–Liouville fractional difference equation:

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

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. 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*

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

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

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

and 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 $y(x_1), \dots, y(x_{N-1})$. The corresponding matrix form is as follows:

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

where the entries A_{ij} of A are

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

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

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

we get an eigenvalue problem with the symmetric matrix $R^{-1}A$. Because of the equivalence of problem (2-5)–(2-6) with 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 $c_1, \dots, c_{N-1}$ such that $\varphi(x_k) = \sum_{i=1}^{N-1} c_i y^i(x_k)$, $1 \le k \le N-1$. Note that

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

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

2B. **Isoperimetric Variational Problems.** In this section we prove two theorems connecting the Sturm–Liouville problem (2-5)–(2-6) with 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 to the first eigenvalue λ_1 of problem (2-5)–(2-6)*. Then y^1 is a minimizer of functional*

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

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

Proof. Suppose that y is a minimizer of J. Then, by Theorem 5 [32], there exists a real constant λ such that y satisfies equation

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

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

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

By summation by parts (2-4)

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

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

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

Any solution to problem (2-9)–(2-10) that satisfies equation (2-11) must be nontrivial since (2-9) holds, so λ must be an eigenvalue. According to Theorem 2.4 there is the least element in the spectrum being eigenvalue λ_1, and the 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 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 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 the case (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 following functions

$$\begin{aligned} \phi: \quad [-\varepsilon,\varepsilon] &\longrightarrow \mathbb{R} \\ h &\longmapsto I[y+h\eta] = \sum_{k=1}^{N} r(x_k)(y(x_k)+h\eta(x_k))^2 \end{aligned}$$

$$\begin{aligned} \psi: \quad [-\varepsilon,\varepsilon] &\longrightarrow \mathbb{R} \\ h &\longmapsto J[y+h\eta] = \sum_{k=1}^{N} \left[p(x_k)\left({}_0\Delta_k^{\alpha}(y(x_k)+h\eta(x_k))\right)^2 + q(x_k)(y(x_k)+h\eta(x_k))^2\right] \end{aligned}$$

and

$$\begin{aligned} \zeta: \quad [-\varepsilon,\varepsilon] &\longrightarrow \mathbb{R} \\ h &\longmapsto R[y+h\eta] = \tfrac{J[y+h\eta]}{I[y+h\eta]}, \end{aligned}$$

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

$$\zeta(0) \le \zeta(h), \ |h| \le \varepsilon,$$

we deduce that

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

Moreover, notice that

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

and

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

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

Therefore

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

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

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

Since η is arbitrary, we have

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

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

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

Similarly to the proof of Theorem 2.5, we can obtain

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

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

$$\lambda \le R[y^i] = \lambda_i \ \forall i \in \{1,\dots,N-1\}$$

we have $\lambda = \lambda_1$. □

Example 2.8. *Let us consider the following problem: minimize*

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

subject to

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

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

$$ {}_k\Delta_{N0}^\alpha\Delta_k^\alpha y(x_k) = \lambda y(x_k), \quad k = 1,\dots,N-1. \tag{2-16}$$

Together with boundary condition $y(x_0) = y(x_N) = 0$ *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*'s are presented in Table 1. Those results are obtained by solving the matrix eigenvalue problem of the form* (2-8).

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's: $1/4, 1/2, 3/4, 1$.

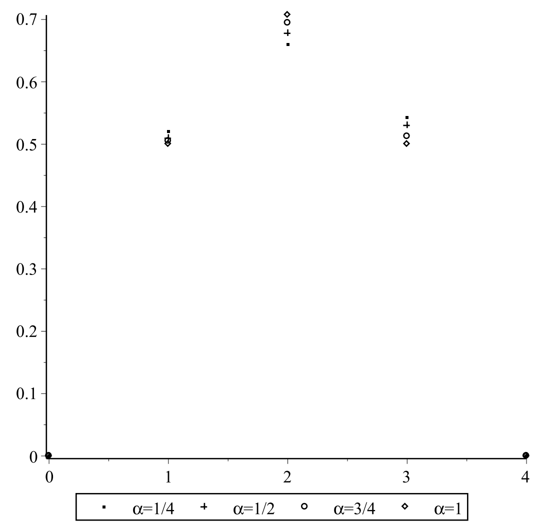

FIGURE 1. The solution to problem (2-14)–(2-15) for different values of α's: $1/4, 1/2, 3/4, 1$.

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: $y_1 = y(x_1), \ldots, y_{N-1} = y(x_{N-1})$ 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's. 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 found by using the first order necessary optimality conditions (Karush–Kuhn–Tucker conditions), that is, by solving the following system of equations:*

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

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's: $1/4, 1/2, 3/4, 1$.

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 [21], 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*

(1) *the left and right Riemann–Liouville fractional derivatives of order α by*

$$ {}_aD_x^\alpha f(x) := \frac{1}{\Gamma(1-\alpha)}\frac{d}{dx}\int_a^x (x-t)^{-\alpha} f(t)dt, $$

and

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

respectively;

(2) *the left and right Caputo fractional derivatives of order α by*

$$ {}_a^CD_x^\alpha f(x) := \frac{1}{\Gamma(1-\alpha)}\int_a^x (x-t)^{-\alpha} f'(t)dt, $$

and

$$ {}_x^CD_b^\alpha f(x) := \frac{-1}{\Gamma(1-\alpha)}\int_x^b (t-x)^{-\alpha} f'(t)dt, $$

respectively.

The Caputo derivative seems more suitable in applications. Let us recall that the Caputo derivative of a constant is zero, whereas for 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 type of conditions. On the other hand the Laplace transform of the Caputo derivative imposes boundary conditions involving the value of 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 a real. The left and right Grünwald–Letnikov fractional derivative of a function f, of order α, is defined as*

$$ {}_a^{GL}D_x^\alpha f(x) := \lim_{h\to 0^+}\frac{1}{h^\alpha}\sum_{k=0}^{\infty}(-1)^k\binom{\alpha}{k} f(x-kh), $$

and

$$ {}_x^{GL}D_b^\alpha f(x) := \lim_{h\to 0^+}\frac{1}{h^\alpha}\sum_{k=0}^{\infty}(-1)^k\binom{\alpha}{k} f(x+kh), $$

respectively.

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

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

rather than $a_i^{(\alpha)}$.

Relations between those three types of derivatives are given below and can be found respectively in [39, 21].

Proposition 3.3. *Let us assume that 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. *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*

$$ {}_a^C D_x^\alpha f(x) = {}_a D_x^\alpha f(x) - \frac{f(a)}{\Gamma(1-\alpha)}(x-a)^{-\alpha} \tag{3-1}$$

and

$$ {}_x^C D_b^\alpha f(x) = {}_x D_b^\alpha f(x) - \frac{f(b)}{\Gamma(1-\alpha)}(b-x)^{-\alpha}.$$

If $f(a) = 0$ or $f(b) = 0$, then ${}_a^C D_x^\alpha f(x) = {}_a D_x^\alpha f(x)$ or ${}_x^C D_b^\alpha f(x) = {}_x D_b^\alpha f(x)$, 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 $j = 0, 1, ..., N$ and some $h > 0$ such that $x_N = b$, we have

$$ {}_a D_{x_j}^\alpha f(x_j) = \frac{1}{h^\alpha} \sum_{k=0}^{j} (w_k^\alpha) f(x_{j-k}) + O(h),$$

$$ {}_{x_j} D_b^\alpha f(x_j) = \frac{1}{h^\alpha} \sum_{k=0}^{N-j} (w_k^\alpha) f(x_{j+k}) + O(h),$$

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

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

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

3A. **Variational Problem.** Consider the following variational problem: to 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

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

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. *([2]) If $\overline{y}$ is a solution to* (3-4)–(3-5)*, then $\overline{y}$ satisfies the following fractional differential equation*

$$\frac{\partial L}{\partial y}(x, y(x), {}^C_a D^\alpha_x y(x)) + {}_x D^\alpha_b \frac{\partial L}{\partial {}^C_a D^\alpha_x y}(x, y(x), {}^C_a D^\alpha_x y(x)) = 0, \quad t \in [a,b]. \tag{3-6}$$

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 verify. Adding to problem (3-4)–(3-5) an integral constraint

$$\int_a^b g(x, y(x), {}^C_a D^\alpha_x y(x))\, dx = K, \tag{3-7}$$

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

$$F := \lambda_0 L(x, y(x), {}^C_a D^\alpha_x y(x)) - \lambda g(x, y(x), {}^C_a D^\alpha_x y(x)), \tag{3-8}$$

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

$$\frac{\partial F}{\partial y}(x, y(x), {}^C_a D^\alpha_x y(x)) + {}_x D^\alpha_b \frac{\partial F}{\partial {}^C_a D^\alpha_x y}(x, y(x), {}^C_a D^\alpha_x y(x)) = 0, \quad t \in [a,b]. \tag{3-9}$$

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

$$\frac{\partial g}{\partial y}(x, y(x), {}^C_a D^\alpha_x y(x)) + {}_x D^\alpha_b \frac{\partial g}{\partial {}^C_a D^\alpha_x y}(x, y(x), {}^C_a D^\alpha_x y(x)) = 0, \quad t \in [a,b], \tag{3-10}$$

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

3A.1. *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

$$\begin{aligned} I[y] &= \sum_{k=1}^{N} \int_{x_{k-1}}^{x_k} L(x, y(x), {}^C_a D^\alpha_x y(x))\, dx \\ &\approx \sum_{k=1}^{N} hL(x_k, y(x_k), {}^C_a D^\alpha_{x_k} y(x_k)) \\ &\approx \sum_{k=1}^{N} hL(x_k, y(x_k), {}^C_a \tilde{D}^\alpha_{x_k} y(x_k)). \end{aligned} \tag{3-11}$$

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

3A.2. *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

$$\Phi(y_1, \ldots, y_{N-1}) := \sum_{k=1}^{N} hL(x_k, y(x_k), {}^C_a \tilde{D}^\alpha_{x_k} y(x_k)) \;\to\; \min,$$

subject to

$$y_0 = y_a \text{ and } y_N = y_b$$

where $y_k := y(x_k)$.

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

$$\frac{\partial \Phi}{\partial y_j} = 0, \quad \forall j = 1, \dots, N-1,$$

we get

$$\frac{\partial L}{\partial y}(x_j, y(x_j), {}^C_a\tilde{D}^\alpha_{x_j} y(x_j)) + \sum_{k=0}^{N-j} \frac{(w_k^\alpha)}{h^\alpha} \frac{\partial L}{\partial {}^C_a D^\alpha_x y}(x_{j+k}, y(x_{j+k}), {}^C_a\tilde{D}^\alpha_{x_{j+k}} y(x_{j+k})) = 0 \tag{3-12}$$

$j = 1, \dots, N-1$. 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 to the variational problem (see [40, Theorem 4.1]). 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

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

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:

*(A)***:** Let $\frac{1}{2} < \alpha < 1$ and p, q, 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 $\beta \leq \alpha - \frac{1}{2}$, on $[a,b]$.

Theorem 3.6. *(*[23]*) Under assumption (A), the fractional Sturm–Liouville Problem* (3-13)–(3-14) *has an infinite increasing sequence of eigenvalues $\lambda_1, \lambda_2, \ldots$, and to each eigenvalue λ_k there is a corresponding continuous eigenfunction y_k which is unique up to a constant factor.*

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

Theorem 3.7. *(*[23]*) Let assumption (A) holds 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 to the first eigenvalue λ_1 of problem (3-13)–(3-14) *and assume that function $D^\alpha_b(p {}^C D^\alpha_a y^1)$ is continuous. Then, y^1 is a minimizer of the following variational functional:*

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

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

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

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

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

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

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

which in the matrix form, may be written as

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

where $Y=[y_1\ y_2\ldots y_{N-1}]$, $y_i=y(x_i)$, and $A=(c_{ik})$, $i=1,2,\ldots,N-1$, $k=1,2,\ldots,N-1$, with $c_{ik}=\begin{cases}\frac{h^{-2\alpha}}{r_\alpha(x_i)}\sum_{j=0}^{N-i}\left(w_j^\alpha\right)^2p(x_{j+i})+\frac{q(x_i)}{r_\alpha(x_i)}, & i=k\\ \frac{h^{-2\alpha}}{r_\alpha(x_i)}\sum_{j=0}^{N-i}\left(w_j^\alpha\right)\left(w_{j+i-k}^\alpha\right)p(x_{j+i}), & i>k,\\ \frac{h^{-2\alpha}}{r_\alpha(x_i)}\sum_{j=k-i}^{N-i}\left(w_j^\alpha\right)\left(w_{j+i-k}^\alpha\right)p(x_{j+i}), & i<k\end{cases}$
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*

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

under the restrictions

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

where $\alpha=3/4$. Since $y(0)=0$, we have ${}_0^CD_x^\alpha y(x)={}_0D_x^\alpha y(x)$. Discretizing the problem, as explained in Section 3A.1, we obtain a finite dimensional constrained optimization problem:

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

subject to

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

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 $\overline{y}=[0,y_1,\ldots,y_{N-1},0]$ 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 (which is the Euler–Lagrange equation for considered variational problem). Figure 2 presents minimizers $\overline{y}$ for $N=5,10,15$.*

N	5	10	15
λ_1	4.603751971	4.491185175	4.426964914

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

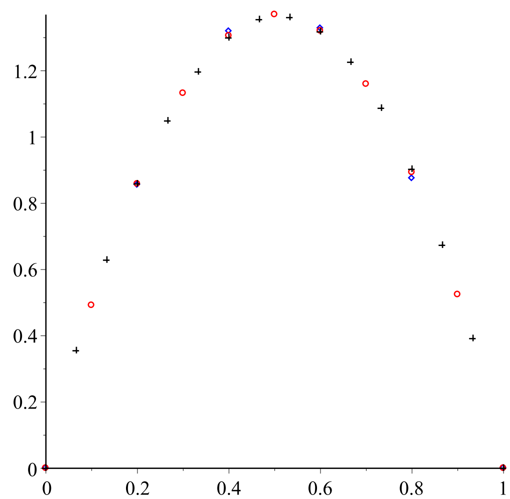

FIGURE 2. Approximation of solutions to problem (3-19)–(3-20) (Method 1): $\diamond(N = 5)$; $\circ(N = 10)$; $+(N = 15)$.

Observe that the unique solution to the Euler–Lagrange equation (cf. (3-10)*) associated to the integral constraint is* $\overline{y}(x) = 0$. *As* $\overline{y}(x) = 0$ *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,

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

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) *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 3 we present the optimal solution for this procedure, that corresponds to the eigenvector associated with the eigenvalue* λ_1.

In Figures 4, 5 and 6 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* $N = 5, 10, 15$.

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 $N = 5, 10, 15$.

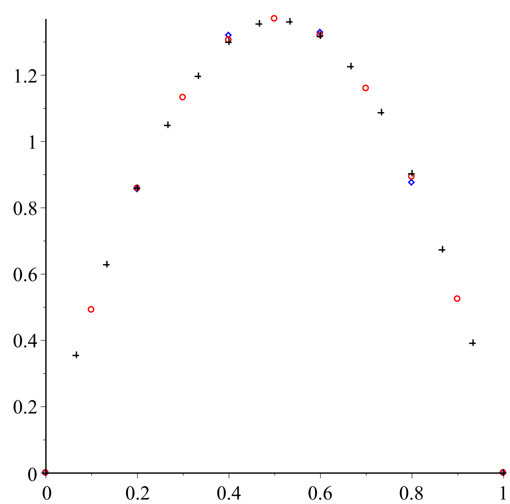

FIGURE 3. Approximation of solutions to problem (3-19)–(3-20) (Method 2): $\diamond(N = 5)$; $\circ(N = 10)$; $+(N = 15)$.

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

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

Note that, under conditions of Theorem 3.7, equation (3-24) *is the Euler–Lagrange equation for isoperimetric problem* (3-19)–(3-20). *Table 3.8 presents approximations of the eigenvalues of* (3-24) *obtained by discretization method 3B.1 for* $N = 5, 10, 20, 40, 80, 160$ *(for* $N =$

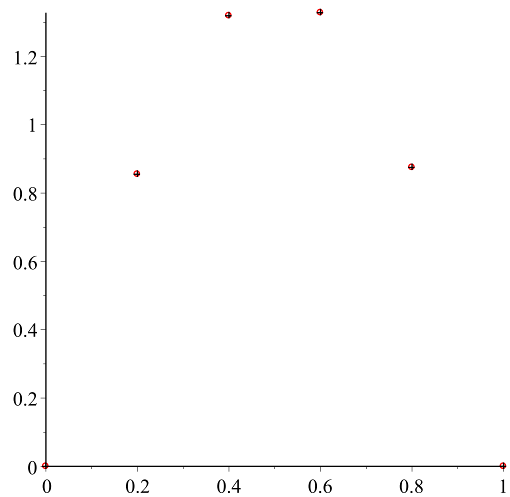

FIGURE 4. $N = 5$: $\circ$(Method 1); $+$(Method 2).

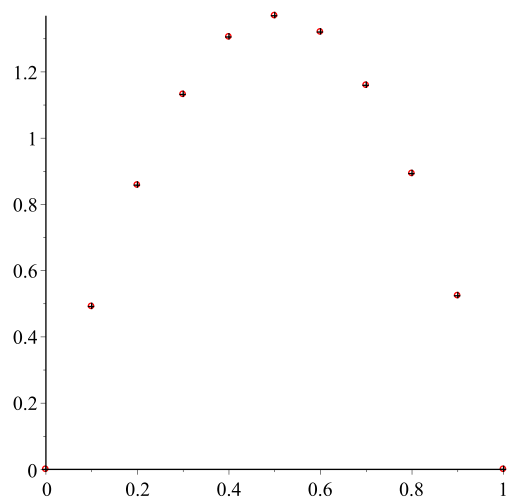

FIGURE 5. $N = 10$: $\circ$(Method 1); $+$(Method 2).

$20, 40, 80, 160$ *only the first 14 eigenvalues are listed). In Figure 3.8 we present normalized eigenfunctions, obtained for* $N = 100$*, corresponding to the eigenvalues* λ_1*,* λ_2*,* λ_3 *and* λ_4*.*

4. Conclusions

Since 1986, when the seminal works were published [37, 44], fractional differential equations have become a popular way to model anomalous diffusion. As it is stated in [33] this type of approach is the most reasonable: the fractional derivative in space codes large particle jumps (that lead to anomalous super-diffusion) 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 [9] and flow in porous media [18]. Many other examples can be found in [33, 34].

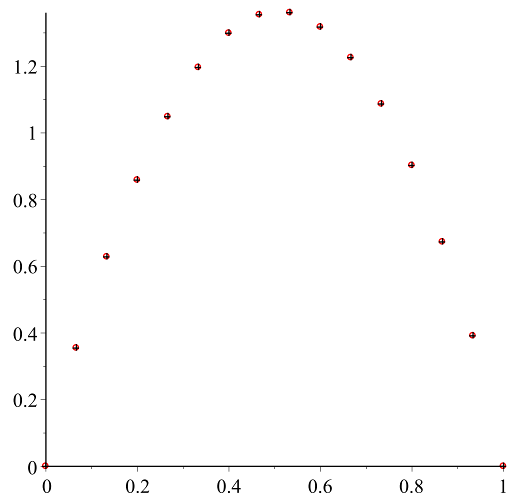

FIGURE 6. $N = 15$: ∘(Method 1); +(Method 2).

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 3B.1.

It was proved in [26] that, under appropriate assumptions, the following space–time fractional diffusion equation

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

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

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

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

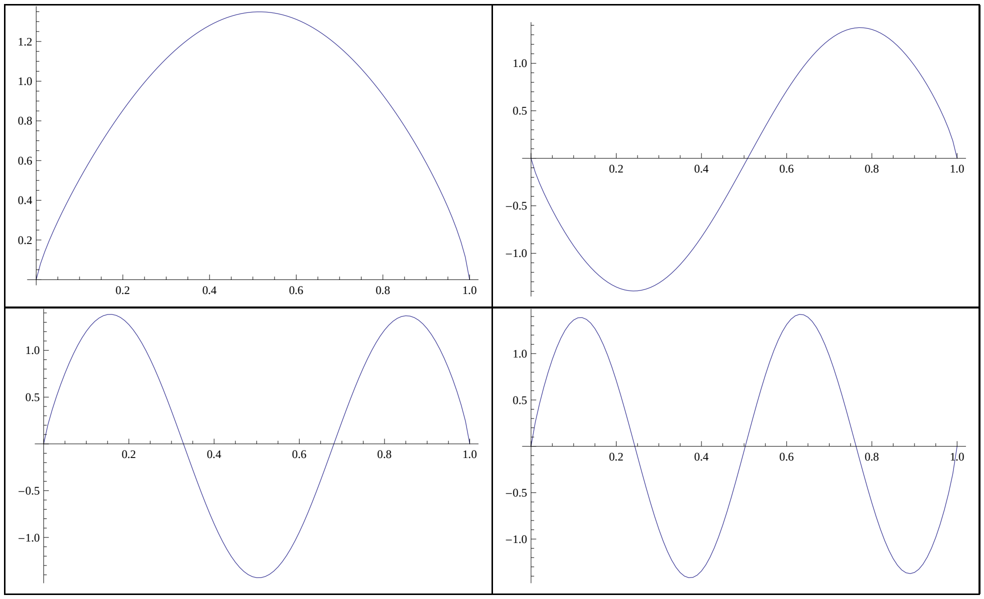

FIGURE 7. Normalized eigenfunctions obtained with $N = 100$, corresponding to the eigenvalues λ_1, λ_2, λ_3 and λ_4 (top left, top right, bottom left and bottom right, respectively).

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 the one-parameter Mittag–Leffler function, y_k and λ_k ($k = 1, 2, \ldots$) 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 be also used to approximate solution 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 those firstly mentioned problems. 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 were used. This type of discretization is most popular in practical application, when solving numerically fractional diffusion equations, due to the fact that codes are mass-preserving [14].

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