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Operational matrix formulation of Legendre LSSVR for Caputo-type integro-differential equations

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This study develops a numerical framework for solving Caputo-type fractional integro-differential equations using a hybrid formulation that integrates Legendre polynomial operational matrices within the Least Squares Support Vector Regression (LSSVR) paradigm. The proposed method reformulates the governing equations by representing all differential, integral, and integral-kernel operators in matrix form, derived from the orthogonality and recurrence properties of Legendre bases. This leads to a fully vectorized constrained optimization problem, subsequently reduced to a symmetric linear system via KarushKuhnTucker conditions. The approach retains the spectral convergence characteristics of orthogonal polynomial methods while incorporating the regularization and flexibility of LSSVR. Numerical experiments on benchmark problems with known solutions demonstrate exponential accuracy and high numerical stability across varying polynomial degrees. This formulation accommodates both Fredholm and Volterra integral structures and directly incorporates Caputo initial conditions without reformulation. The method is compatible with higher-dimensional extensions and adaptable to various kernel approximations.

Keywords: Fractional Calculus; Operational Matrix; Legendre Polynomials.

1. Introduction

Integro-differential equations, encompassing both the Fredholm and Volterra varieties, arise naturally in the modeling of anomalous diffusion processes, viscoelastic materials, population dynamics, and feedback control systems[10, 9, 17]. Their combined differential and integral operators capture memory effects and nonlocal interactions that are impossible to describe with classical integer-order models.

In recent decades, fractional calculus has provided the theoretical underpinning for extending classical differential operators to fractional orders, typically via Caputo or RiemannLiouville definitions [20, 18]. These operators introduce hereditary properties into the governing equations, enabling the order of differentiation to assume non-integer values and thereby richer dynamics. However, the nonlocal nature of fractional derivatives, where every evaluation depends on the entire solution history, poses significant challenges for both computational cost and stability in large-scale simulations.

Despite the wealth of analytical techniques developed over the years, most of these models do not admit closed-form solutions, which necessitates the design of efficient and high-accuracy numerical schemes to approximate their behavior. Various numerical methods for addressing such problems have been proposed [15, 16, 11]. Based on these approaches, the present work aims to extend their application to more complex problem classes using the Least Squares Support Vector Regression (LSSVR) framework.

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Spectral methods based on orthogonal polynomial expansions have emerged as leading contenders for the discretization of integro-differential equations, due to their exponential convergence rates for smooth solutions and the ability to convert differentiation and integration into sparse matrix operations. Among these, Legendre polynomialbased schemes stand out: their orthogonality on the canonical interval minimizes numerical error accumulation.

Based on these advances, we propose an integrated framework that embeds Legendre operational matrices for Caputo derivatives, spatial derivatives, and integral operators directly into the LSSVR formulation. By expressing all operators in a unified matrix format, the consequent hybrid solver transforms the problem into a single, fully matrix-based optimization. This approach retains the spectral accuracy and computational efficiency of classical operational-matrix methods while leveraging the adaptability and data-driven regularization of LSSVR [14].

The rest of the paper is organized as follows: In Section 2, we explain the Legendre approximation and how to obtain its coefficients. In Section 3, we discuss fractional calculus, including the Caputo fractional derivative. Finally, in Section 4, we discuss the desired formula and the new method, which is a combination of approximation methods with a machine learning method. Also in Section 5 presents experimental results, evaluation tables, and related diagrams. Finally, Section 6 examines the value of the introduced method.

2. Legendre Polynomials

In the field of numerical analysis and scientific computing, the ability to accurately represent complex functions is paramount. Among the diverse array of function approximation techniques, those leveraging orthogonal polynomials stand out for their elegance and computational efficiency. Prominent among these are Legendre polynomials, which form the basis of a highly effective approximation strategy, particularly over finite intervals.

2.1. Defining the Legendre Polynomials

Legendre polynomials, denoted by $P_n(x)$, constitute a sequence of orthogonal polynomials. They are specifically defined on the interval $[-1,1]$ and are the solutions to the Legendre differential equation [1, 19, 5]:

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + n(n+1)y = 0 \tag{1}$$

where n is a non-negative integer representing the degree of the polynomial. Each $P_n(x)$ is a polynomial of degree n.

The first few Legendre polynomials are:

- $P_0(x) = 1$
- $P_1(x) = x$
- $P_2(x) = \frac{1}{2}(3x^2 - 1)$
- $P_3(x) = \frac{1}{2}(5x^3 - 3x)$
- $P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$

Legendre polynomials are orthogonal with respect to the weight function $w(x) = 1$ over the interval $[-1,1]$. Mathematically, this means:

$$\int_{-1}^{1} P_m(x)P_n(x)dx = \begin{cases} 0 & \text{if } m \neq n \\ \frac{2}{2n+1} & \text{if } m = n \end{cases} \tag{2}$$

This orthogonality simplifies the process of determining coefficients in an approximation, as each coefficient can be calculated independently. Legendre polynomials can be generated very efficiently using a simple recurrence relation:

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \tag{3}$$

Starting with $P_0(x) = 1$ and $P_1(x) = x$, one can generate all higher-order polynomials iteratively. This property is invaluable for computational implementations.

An explicit formula for $P_n(x)$ is given by Rodrigues' formula:

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n \tag{4}$$

This formula provides a direct way to compute any Legendre polynomial, particularly useful for theoretical derivations. Also, Legendre polynomials are normalized such that $P_n(1) = 1$ for all n. This helps in standardizing their use.

All n roots of $P_n(x)$ are real, distinct, and lie within the interval $(-1,1)$. Furthermore, the roots of $P_n(x)$ interlace with the roots of $P_{n+1}(x)$, a property important for numerical integration techniques like Gaussian quadrature. Although naturally defined on $[-1,1]$, Legendre polynomials can be easily adapted to approximate functions on any arbitrary interval $[a,b]$ through a simple linear transformation:

$$x = \frac{2t-(a+b)}{b-a} \tag{5}$$

This maps a variable t from $[a,b]$ to x in $[-1,1]$, allowing for broad applicability.

2.2. Legendre Approximation

The core idea of Legendre approximation is to represent a sufficiently well-behaved function $f(x)$ as a finite series of Legendre polynomials:

$$f(x) \cong P_x^{\top} c = \sum_{n=0}^{N} c_n P_n(x) \tag{6}$$

Here, N is the maximum degree of the polynomial used in the approximation, often referred to as the truncation order. The goal is to find the coefficients c_n that make best approximation of $f(x)$ in some sense.

To find the coefficients c_k, we multiply both sides of the approximation by $P_k(x)$ and integrate over $[-1, 1]$:

$$\int_{-1}^{1} f(x)P_k(x)dx = \int_{-1}^{1} \left(\sum_{n=0}^{N} c_n P_n(x) \right) P_k(x)dx$$
$$\int_{-1}^{1} f(x)P_k(x)dx = \sum_{n=0}^{N} c_n \int_{-1}^{1} P_n(x)P_k(x)dx$$

Due to orthogonality, all terms in the sum on the right-hand side become zero except when $N = k$. This leaves us with:

$$\int_{-1}^{1} f(x)P_k(x)dx = c_k \int_{-1}^{1} (P_k(x))^2 dx$$
$$\int_{-1}^{1} f(x)P_k(x)dx = c_k \left(\frac{2}{2k+1} \right)$$

Solving for c_k, we get the explicit formula for the Fourier-Legendre coefficients:

$$c_k = \frac{2k+1}{2} \int_{-1}^{1} f(x)P_k(x)dx \tag{7}$$

This means that each coefficient can be computed independently, making the process highly parallelizable and efficient.

3. Fractional Calculus

Classic calculus deals with derivatives and integrals of integer orders. However, many complex systems in nature and engineering exhibit behaviors that are not adequately described by integer-order models. This is where Fractional Calculus steps in, extending the concept of differentiation and integration to non-integer (arbitrary) orders. It provides a powerful mathematical framework to model phenomena exhibiting memory and history-dependent properties, which are common in viscoelasticity, anomalous diffusion, control theory. While the idea of fractional derivatives dates back to Leibniz and L'Hopital, its rigorous development and application have gained significant traction in recent decades. Several definitions of fractional derivatives exist, including Riemann-Liouville, Grnwald-Letnikov, and Caputo. Each definition has its own strengths and weaknesses, but for modeling real-world physical processes, the Caputo fractional derivative often emerges as the preferred choice due to its direct compatibility with standard initial and boundary conditions. The primary advantage of the Caputo derivative over other definitions (such as the Riemann-Liouville derivative) lies in its ability for the direct inclusion of classical integer-order initial conditions into the fractional differential equation.

3.1. Definition of the Caputo Fractional Derivative

For a function $f(t)$ and a fractional order $\alpha > 0$, the Caputo fractional derivative of order α starting from a is defined as:

$${}_a^C D_t^{\alpha} f(t) = {}_a^{RL} D_t^{-(n-\alpha)} f^{(n)}(t) = \frac{1}{\Gamma(n-\alpha)} \int_a^t \frac{f^{(n)}(t)}{(t-t)^{\alpha-n+1}} dt \tag{8}$$

where $n-1 < \alpha \le n$, and n is the smallest integer greater than or equal to α. Here, $\Gamma(\cdot)$ is the Gamma function, which generalizes the factorial function to real and complex numbers. When $\alpha = n$ (an integer order), the Caputo derivative reduces to the standard integer-order derivative:

$${}_a^C D_t^{n} f(t) = f^{(n)}(t) \tag{9}$$

For $\alpha = 0$, it is simply $f(t)$. A commonly used case is the Caputo derivative starting from $t = 0$, often denoted as D_0^{α}.

3.2. Key Properties of the Caputo Fractional Derivative

The Caputo derivative of a constant is zero, just like the integer-order derivative, provided $\alpha > 0$.

$$ {}_a^C D_t^{\alpha} C = 0, \quad \text{for } \alpha > 0 \text{ and } C \text{ is a constant.} $$

This property is essential for consistency with physical models where constant quantities do not change over time. While different, there's a relationship between the Caputo derivative and the Riemann-Liouville fractional derivative (${}_a^C D_t^{\alpha} f(t) = I_a^{n-\alpha} \frac{d^n}{dt^n} f(t)$ where I is the fractional integral). This connection is useful for theoretical analysis. For power functions, the Caputo derivative is given by:

$$ {}_a^C D_t^{\alpha} (t-a)^{\beta} = \begin{cases} \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha+1)} (t-a)^{\beta-\alpha} & \text{if } \beta > n-1 \\ 0 & \text{if } \beta \in \{0, 1, \ldots, n-1\} \end{cases} $$

This explicitly shows how derivatives of lower-order powers become zero, aligning with integer-order calculus where derivatives of polynomials eventually become zero.

3.2.1. Operational Matrices In function approximation tasks involving differential and integral equations, the derivatives and integrals of Legendre polynomials naturally arise. In matrix notation, the derivatives of Legendre polynomials can be expressed in terms of the polynomials themselves as follows [6, 7]:

$$ \frac{d^{\alpha}}{dx^{\alpha}} P(x) = \mathcal{D}^{\alpha} \, P(x), $$

where $P(x)$ is an $(N+1)$-dimensional vector of Legendre polynomials, and the matrix $\mathcal{D}^{\alpha}$ is given by

$$ \mathcal{D}_{i,j}^{\alpha} = \frac{\left\langle \frac{\mathrm{d}^{\alpha}}{\mathrm{d}x^{\alpha}} P_i(x), P_j(x) \right\rangle}{\langle P_j(x), P_j(x) \rangle}, \qquad i, j = 0, 1, 2, \ldots, N. \tag{10} $$

4. New Method

This paper addresses the numerical solution of fractional partial integro-differential equations of Fredholm or Volterra type, expressed as

$$ {}_0^C D_t^{\alpha} U(x) = f(x) + \int_{\Omega} K(x,s) U(s) \, \mathrm{d}s, \tag{11} $$

subject to compatible initial and boundary conditions. Here, $x \in \mathbb{R}$ denotes the spatial coordinate in n dimensions, $t \in \mathbb{R}^+$ denotes time, and $U : \mathbb{R}^+ \to \mathbb{R}$ is a sufficiently smooth unknown function. The integral kernel $K : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}$ is assumed to possess sufficient smoothness over problem domain Ω. the operator ${}_0^C D_t^{\alpha}$ denotes the Caputo fractional derivative of fixed real number α.

In this approach, the unknown solution to the integro-differential equation (11) is represented by an approximate expression.

$$ U_N(x) \cong P_x^{\top} v = \sum_{k=0}^{N} v_k \, P_k(x), \tag{12} $$

where v_k are the weights and $P_k(x)$ are the Legendre polynomials. In this approach, we propose considering the primal form of LSSVR in a vectorized format:

$$ \begin{aligned} \min_{\omega e} \quad & \frac{1}{2} \omega^{\top} \omega + \frac{\lambda}{2} e^{\top} e \\ \text{s.t.} \quad & {}_0^C D^{\alpha} U_M(x) - \int_{\Omega} K(x,s) U_M(s) ds - f(x) = e. \end{aligned} \tag{13} $$

Now, we utilize the vectorized format of the Legendre approximation from (14) along with the operational matrices to simplify the constraints. Consequently, the constraints in (13) can be reformulated as [2]:

$$ \begin{aligned} P_{\hat{x}}^{\top} \mathcal{D}^{\alpha} v - P_{\hat{x}}^{\top} R \mathcal{H} v - P_{\hat{x}}^{\top} \mathfrak{q} &= e, \\ P_{\hat{x}}^{\top} \left(\left[\mathcal{D}^{\alpha} - R\mathcal{H} \right] v - \mathfrak{q} \right) &= e, \\ \mathcal{B} \left(\left[\mathcal{D}^{\alpha} - R\mathcal{H} \right] v - \mathfrak{q} \right) &= e, \end{aligned} $$

where $\mathcal{D}^{\alpha}$ is defined in, $\mathfrak{q}_N$ and $R_{N\times N}$ for $N = M + 1$ are obtained by approximating $f(\cdot)$ and $K(\cdot, \cdot)$ using 1D and 2D Legendre approximations via the least squares method [8]:

$$f_M(x) \cong P_x^{\top}\ \mathfrak{q} = \sum_{i=0}^{M} \mathfrak{q}_i\ P_i(x), \tag{14}$$

and

$$K_N(x, \hat{x}) = K_N(\boldsymbol{x}) \cong P_x^{\top}\ R\ P_{\hat{x}} = \sum_{i=0}^{N}\sum_{j=0}^{N} R_{i,j}\ P_{i,j}(x), \tag{15}$$

and:

$$\mathcal{H}_{N\times N} = \int_{\Omega} P_s P_s^{\top}\, ds, \tag{16}$$

is the symmetric quadrature matrix where

$$\mathcal{H}_{m,n} = \int_{-1}^{1} P_m(x)P_n(x)dx = \begin{cases} 0 & \text{if } m \neq n \\ \frac{2}{2n+1} & \text{if } m = n. \end{cases}$$

Here, $\mathcal{B}_{j,k} = P_k(\hat{x}_j)$ for $j = 1, \dots, N$ and $k = 0, \dots, M$.

We then construct the Lagrangian function:

$$\theta(v, e, \mathfrak{z}) = \frac{1}{2}\omega^{\top}\omega + \frac{\lambda}{2}e^{\top}e - \mathfrak{z}^{\top}\left[\mathcal{B}\left(\left[\mathcal{D}^{\alpha} - R\mathcal{H}\right]c - \mathfrak{q}\right) - e\right].$$

Solving the Karush-Kuhn-Tucker conditions yields the dual form as a positive semi-definite system of equations:

$$\left[A + \frac{1}{\lambda}I\right]\mathfrak{z} = \mathcal{B}\mathfrak{q}, \tag{17}$$

where $\mathfrak{q}$ is the set of Legendre coefficients for approximating $f(x)$, $A = \Pi^{\top}\Pi$, and the matrix Π can be calculated using the operational matrices of the Legendre polynomials:

$$\Pi_{N\times N} = \left[\mathcal{B}\left[\mathcal{D}^{\alpha} - R\mathcal{H}\right]\right]^{\top}. \tag{18}$$

Here, the weights v are calculated as $v = \Pi\mathfrak{z}$. The approximation for the problem can then be derived using Equation (13). The full algorithm of this method is presented in 1.

Algorithm 1 OPM-LSSVR for Fractional Integro-Differential Equations

Require: Fractional order α, forcing function $f(x)$, integral kernel $K(x, s)$, polynomial truncation order N, regularization parameter λ, problem domain $[a, b]$.

Ensure: Approximate solution $U_N(x)$.

1: Define the linear transformation $y = \frac{2x-(a+b)}{b-a}$ to map $x \in [a, b]$ to $y \in [-1, 1]$. All subsequent calculations involving Legendre polynomials, operational matrices, and integral coefficients are performed on this transformed domain $y \in [-1, 1]$.
2: Choose $N + 1$ collocation points $\hat{y}_j \in [-1, 1]$ (e.g., uniformly distributed points or Legendre-Gauss-Lobatto points).
3: Construct the Legendre polynomial basis vector $\mathbf{P}(y) = [P_0(y), P_1(y), \dots, P_N(y)]^T$.
4: Compute the Caputo fractional differentiation operational matrix $\mathcal{D}^{\alpha}$ of size $(N + 1) \times (N + 1)$ for Legendre polynomials on $[-1, 1]$.
5: Compute the symmetric quadrature matrix $\mathcal{H}$ of size $(N + 1) \times (N + 1)$ for Legendre polynomials over $[-1, 1]$, where $\mathcal{H}_{m,n} = \int_{-1}^{1} P_m(y)P_n(y)dy$.
6: Construct the evaluation matrix $\mathcal{B}$ of size $(N + 1) \times (N + 1)$ where $\mathcal{B}_{j,k} = P_k(\hat{y}_j)$ for $j, k = 0, \dots, N$.
7: Approximate the transformed forcing function $f(y)$ using Legendre series to obtain the coefficient vector $\mathfrak{q}$ of size $(N + 1)$. That is, $f(y) \approx \mathbf{P}(y)^T\mathfrak{q}$.
8: Approximate the transformed kernel $K(y_1, y_2)$ using a 2D Legendre series to obtain the coefficient matrix R of size $(N + 1) \times (N + 1)$. That is, $K(y_1, y_2) \approx \mathbf{P}(y_1)^T R\mathbf{P}(y_2)$.
9: Formulate the system matrix Π: $\Pi = \mathcal{B}(\mathcal{D}^{\alpha} - R\mathcal{H})$.
10: Form the system matrix for the dual problem: $A = \Pi^{\top}\Pi$.
11: Solve the linear system $\left(A + \frac{1}{\lambda}I\right)\mathfrak{z} = \mathcal{B}\mathfrak{q}$ for the dual variable vector $\mathfrak{z}$.
12: Calculate the primal coefficient vector $v = \Pi\mathfrak{z}$.
13: **return** The approximate solution $U_N(x) = \mathbf{P}(y(x))^T v = \sum_{k=0}^{N} v_k P_k(y(x))$.

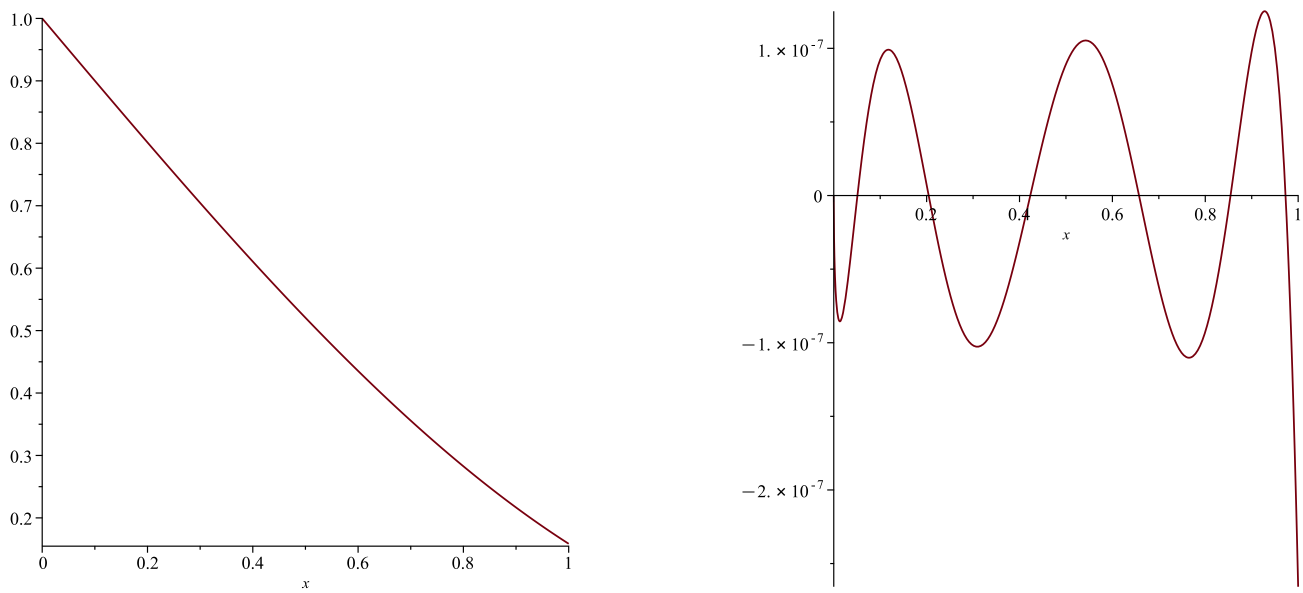
5. Examples

5.1. Example 1

Consider the equation (11) with $\alpha = 0.5$, $K(x,t) = x - t$, exact solution $U(x) = 1 - sin(x)$ with appropriate function $f(x)$. The numerical results, in terms of Mean Absolute Error (MAE), of this problem using $\lambda = 10^{15}$, are reported in Table (1). The predicted solution is drawn in Figure (1). The problem is solved in less than a second by employing the Cholesky decomposition algorithm.

x	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
M								
3	7.97e-05	5.38e-05	1.71e-04	2.09e-04	1.41e-04	9.60e-06	1.64e-04	1.79e-04
5	3.56e-07	2.09e-07	2.32e-07	4.16e-07	1.14e-07	3.52e-07	3.48e-07	2.61e-07
7	1.48e-11	4.20e-10	1.09e-10	4.77e-10	5.91e-11	4.72e-10	1.85e-10	2.39e-10
9	2.57e-13	2.54e-13	5.79e-14	3.23e-13	1.78e-13	1.84e-13	3.22e-13	3.02e-13
11	7.91e-17	2.03e-17	8.07e-17	1.55e-16	1.29e-16	4.18e-17	2.71e-17	6.52e-18

Table 1. MAE of OPM-LSSVR for solving Example (5.1).



(a) Predicted solution (b) Error

Figure 1. Predicted solution of Example 5.1 and its residual function with $M = 12$.

5.2. Example 2

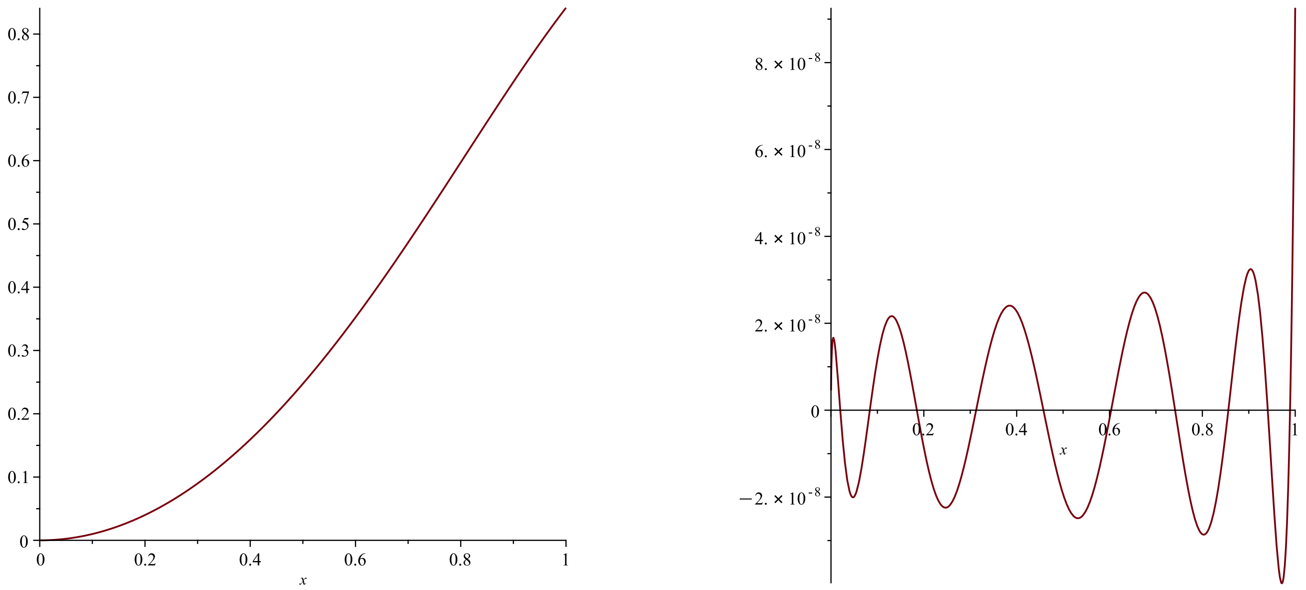
Observe the equation (11) that $\alpha = 0.5$, $K(x,t) = (x^4 + t^2)^{3/2}$, exact solution $U(x) = sin(x^2)$ suitable function $f(x)$. The computational result related to this problem is reported in Table (2). Predicted solution is illustrated in Figure (2). The problem is solved in less than a second by using the Cholesky decomposition algorithm and setting $\lambda = 10^{14}$.

6. Conclusion

This paper introduces a numerical method based on Least Squares Support Vector Regression utilizing the Legendre operational matrix for solving integro-differential equations with fractional derivatives. By employing orthogonal Legendre polynomials and leveraging their operational matrix properties for differentiation, integration, and integral kernels, a novel formulation is developed that models all primary operators of the problem in a unified matrixvector framework. The proposed approach combines the spectral accuracy of Legendre-based methods with the flexibility of the data-driven LSSVR model, enabling the accurate and computationally efficient solution of nonlinear and fractional problems. Numerical results on various benchmark problems

x	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
M								
4	3.55e-04	9.16e-04	6.12e-04	2.78e-04	1.04e-03	1.01e-03	1.08e-04	7.30e-04
6	1.30e-05	9.95e-06	1.93e-05	9.58e-07	2.03e-05	5.51e-06	2.28e-05	2.77e-07
8	1.95e-07	3.68e-08	2.41e-07	7.57e-08	2.45e-07	1.32e-07	8.46e-08	2.07e-07
10	1.52e-09	4.13e-09	4.86e-09	5.26e-10	4.01e-09	5.79e-09	3.36e-09	3.59e-09
12	1.82e-11	1.99e-11	1.58e-11	7.64e-12	5.47e-12	1.08e-11	1.42e-11	5.14e-12

Table 2. MAE of OPM-LSSVR for solving Example (5.2).



(a) Predicted solution

(b) Error

Figure 2. Predicted solution of Example 5.2 and its residual function with $M = 11$.

demonstrate that the method exhibits rapid (exponential) convergence with respect to the polynomial expansion order and offers greater stability and efficiency compared to classical numerical techniques. Selecting training points based on the roots of Legendre polynomials improves matrix conditioning and enhances the numerical stability of the algorithm. The computational complexity of the method mainly depends on the expansion order and the problems dimensionality, both of which can be mitigated through optimized matrix solvers. Additional advantages include full compatibility with initial and boundary conditions in problems involving the Caputo fractional derivative, as well as extensibility to higher-dimensional domains and both Fredholm- and Volterra-type equations. Ultimately, this study demonstrates that integrating the spectral approximation capabilities of Legendre polynomials with the regularized, data-centric structure of LSSVR yields a powerful, accurate, and flexible tool for solving integro-differential equations, including those of fractional types. Future directions include extending the method to more complex geometries, improving hyperparameter selection, and incorporating physics-informed neural networks [13, 3, 4, 12].

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