A Diagonalized Legendre Rational Spectral Method for Problems on the Whole Line

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Abstract. A diagonalized Legendre rational spectral method for solving second and fourth order differential equations are proposed. Some Fourier-like Sobolev orthogonal basis functions are constructed which lead to the diagonalization of discrete systems. Accordingly, both the exact solutions and the approximate solutions can be represented as infinite and truncated Fourier series. Numerical results demonstrate the effectiveness of this approach.

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1 Introduction

Many science and engineering problems are set in unbounded domains, such as fluid flows in an infinite strip, nonlinear wave equations in quantum mechanics and so on. How to accurately and efficiently solve such problems is a very important and difficult subject, since the unboundedness causes considerable theoretical and practical challenges. There are several ways for their numerical simulations. Usually we restrict calculations to some bounded subdomains and impose certain artificial boundary conditions. It is easy to be performed, but it lowers the accuracy sometimes. The second way is to use spectral method associated with some orthogonal systems on the unbounded domains, such as the Laguerre and Hermite spectral method [1, 2, 5, 6, 8–10, 13, 16–19]. However, since the Laguerre/Hermite Gauss points are too concentrated near zero, the approximation results are usually not ideal, especially where the points are far away from zero. The third method is to change original problems by variable transformations to certain singular problems on finite intervals, and then use Jacobi approximation to resolve the
resulting problems [7]. The fourth effective method is to use algebraically mapped Legendre, Chebyshev or Jacobi functions to approximate the differential equations, i.e., the so-called Legendre, Chebyshev or Jacobi rational spectral method [3,4,11,12,21,22]. Compared with the first three methods, we prefer the last way, since the distribution of the Gauss points is more reasonable than that of Laguerre and Hermite Gauss points.

As is well known, the utilization of Legendre rational functions usually leads to a highly sparse algebraic system (a nine-diagonal matrix for second order problems and a seventeen-diagonal matrix for fourth order problems), the condition numbers increase as $O(N^2)$ for the second order problem and $O(N^4)$ for the fourth order problem. However, in many cases, researchers still want a set of Fourier-like basis functions for a diagonalized algebraic system [14, 15, 20]. Motivated by [14, 15, 20], the main purpose of this paper is to construct the Fourier-like Sobolev orthogonal basis functions and propose the diagonalized Legendre rational spectral method for second and fourth problems on the whole line.

The main advantages of the suggested algorithm include: (i) The exact solutions and the approximate solutions can be represented as infinite and truncated Fourier series, respectively; (ii) The condition numbers for the resulting algebraic systems are equal to 1; (iii) The computational cost is much less than that of the classical Legendre rational spectral method.

This paper is organized as follows. In Section 2, we introduce the modified Legendre rational functions and its basic properties. In Section 3, we construct the Sobolev orthogonal Legendre rational functions corresponding to the second order elliptic equation, the fourth order elliptic equation and the nonlinear heat equation, and propose the diagonalized Legendre rational spectral methods. Some numerical results are presented in Section 4 to demonstrate the effectiveness and accuracy.

## 2 Modified Legendre rational functions

We first recall the Legendre polynomials. Let $I = \{y \mid -1 < y < 1\}$ and $L_k(y)$ be the Legendre polynomial of degree $k$, which is the eigenfunction of the singular Sturm-Liouville problem:

$$
\partial_y((1-y^2)\partial_y L_k(y)) + k(k+1)L_k(y) = 0, \quad k \geq 0.
$$

(2.1)

The set of all Legendre polynomials forms a complete $L^2(I)$-orthogonal system, namely,

$$
\int_I L_k(y)L_l(y)dy = \frac{2}{2k+1}\delta_{k,l},
$$

(2.2)

where $\delta_{k,l}$ is the Kronecker function. By virtue of (2.1) and (2.2), we have

$$
\int_I \partial_y L_k(y)\partial_y L_l(y)(1-y^2)dy = \frac{2k(k+1)}{2k+1}\delta_{k,l}.
$$

(2.3)
Moreover, for any $k \geq 1$, the following recurrence relations are satisfied with $L_0(y) = 1$ and $L_1(y) = y$,

\[
\begin{align*}
(k+1)L_{k+1}(y) &= (2k+1)yL_k(y) - kL_{k-1}(y), \\
(2k+1)L_k(y) &= \partial_y L_{k+1}(y) - \partial_y L_{k-1}(y), \\
(2k+1)(1 - y^2)\partial_y L_k(y) &= k(k+1)(L_{k-1}(y) - L_{k+1}(y)).
\end{align*}
\]  

(2.4)

Besides, $L_k(\pm 1) = (\pm 1)^k$ and $\partial_y L_k(\pm 1) = \frac{1}{2}(\pm 1)^{k+1}k(k+1)$.

We next recall the modified Legendre rational functions. Let $\Lambda = \{x \mid -\infty < x < \infty\}$ and $(u, v)$ be the inner product of the space $L^2(\Lambda)$. The modified Legendre rational function of degree $k$ is defined by (cf. [21])

\[
R_k(x) = (x^2 + 1)^{-\frac{3}{2}}L_k\left(\frac{x}{\sqrt{x^2 + 1}}\right), \quad x \in \Lambda, \quad k \geq 0.
\]  

(2.5)

For convenience, let $R_k(x) \equiv 0$ for any integer $k \leq 0$. Due to (2.4), the modified Legendre rational functions satisfy the following recurrence relations with $R_0(x) = (x^2 + 1)^{-\frac{3}{2}}$, $R_1(x) = x(x^2 + 1)^{-\frac{3}{2}}$,

\[
\begin{align*}
(k+1)R_{k+1}(x) &= (2k+1)\frac{x}{\sqrt{x^2 + 1}}R_k(x) - kR_{k-1}(x), \quad k \geq 1, \\
(2k+1)R_k(x) &= (x^2 + 1)^{\frac{3}{2}}(\partial_x((x^2 + 1)^{\frac{3}{2}}R_{k+1}(x))) - \partial_x((x^2 + 1)^{\frac{3}{2}}R_{k-1}(x)), \quad k \geq 1, \\
\partial_x((x^2 + 1)^{\frac{3}{2}}R_k(x)) &= \frac{k(k+1)}{2k+1}(x^2 + 1)^{\frac{3}{2}}(R_{k-1}(x) - R_{k+1}(x)), \quad k \geq 1.
\end{align*}
\]  

(2.6) (2.7) (2.8)

The set of $\{R_k(x)\}_{k \geq 0}$ forms a complete $L^2(\Lambda)$-orthogonal system,

\[
\int_\Lambda R_k(x)R_l(x)dx = \frac{2}{2k+1}\delta_{k,l}.
\]  

(2.9)

Moreover, by (2.3) we know that the functions $\partial_x((x^2 + 1)^{\frac{3}{2}}R_k(x))$ are mutually orthogonal with respect to the weight function $\chi_1(x) = (x^2 + 1)^{\frac{3}{2}}$, 

\[
\int_\Lambda \partial_x((x^2 + 1)^{\frac{3}{2}}R_k(x))\partial_x((x^2 + 1)^{\frac{3}{2}}R_l(x))\chi_1(x)dx = \frac{2k(k+1)}{2k+1}\delta_{k,l}.
\]  

(2.10)

**Lemma 2.1.** For any $k \geq 0$, we have

\[
\partial_x^2R_k(x) = -\frac{k(k-1)(k-2)(k-3)}{4(2k-3)(2k+1)}R_{k-4}(x) + \frac{k(k-1)(2k-1)}{4(2k+1)}R_{k-2}(x) - \frac{3(k^4 + 2k^3 - 2k^2 - 3k - 3)}{2(2k-3)(2k+5)}R_k(x) + \frac{(k+1)(k+2)(2k+3)}{4(2k+1)}R_{k+2}(x) - \frac{(k+1)(k+2)(k+3)(k+4)}{4(2k+1)(2k+5)}R_{k+4}(x),
\]  

(2.11)
and
\[ \partial_x^4 R_k(x) = \frac{k(k+1)}{2k+1}(x^2+1)^{-\frac{5}{2}} \left( \frac{k(k+1)}{2k+1} (R_{k-1}(x) - R_{k+1}(x)) - \frac{3}{2(x^2+1)} R_{k-1}(x) \right) \]
\[ = \frac{k}{2k+1} (x^2+1) \frac{1}{2} (\partial_x (x^2+1)^{\frac{3}{2}} R_k(x)) - \partial_x ((x^2+1)^{\frac{3}{2}} R_{k-2}(x)) \]
\[ - \frac{k+1}{2k+1} (x^2+1)^{\frac{3}{2}} \partial_x ((x^2+1)^{\frac{3}{2}} R_{k+2}(x)) - \partial_x ((x^2+1)^{\frac{3}{2}} R_k(x)) \]
\[ = - \frac{k+1}{2k+1} (x^2+1)^{\frac{3}{2}} \partial_x ((x^2+1)^{\frac{3}{2}} R_{k-2}(x)) + \frac{1}{2} (x^2+1)^{\frac{3}{2}} \partial_x ((x^2+1)^{\frac{3}{2}} R_k(x)) \]
\[ - \frac{k+1}{2k+1} (x^2+1)^{\frac{3}{2}} \partial_x ((x^2+1)^{\frac{3}{2}} R_{k+2}(x)). \]

Proof. By (2.8), (2.6) and (2.7), we derive that

\[ \partial_x R_k(x) = \frac{k(k+1)}{2k+1}(x^2+1)^{-\frac{1}{2}} \left( \frac{k(k+1)}{2k+1} (R_{k-1}(x) - R_{k+1}(x)) - \frac{3}{2(x^2+1)} R_{k-1}(x) \right) \]
\[ = \frac{k}{2k+1} (x^2+1) \frac{1}{2} (\partial_x (x^2+1)^{\frac{3}{2}} R_k(x)) - \partial_x ((x^2+1)^{\frac{3}{2}} R_{k-2}(x)) \]
\[ - \frac{k+1}{2k+1} (x^2+1)^{\frac{3}{2}} \partial_x ((x^2+1)^{\frac{3}{2}} R_{k+2}(x)) - \partial_x ((x^2+1)^{\frac{3}{2}} R_k(x)) \]
\[ = - \frac{k+1}{2k+1} (x^2+1)^{\frac{3}{2}} \partial_x ((x^2+1)^{\frac{3}{2}} R_{k-2}(x)) + \frac{1}{2} (x^2+1)^{\frac{3}{2}} \partial_x ((x^2+1)^{\frac{3}{2}} R_k(x)) \]
\[ - \frac{k+1}{2k+1} (x^2+1)^{\frac{3}{2}} \partial_x ((x^2+1)^{\frac{3}{2}} R_{k+2}(x)). \]
Next, denote by \( A = (a_{kl})_{0 \leq k, l \leq N} \) the matrix with the element \( a_{kl} = (\partial_x R_k, \partial_x R_l) \). By using (2.13) and (2.10), we can deduce readily the nonzero elements of matrix \( A \) as follows,

\[
a_{kk} = \frac{3(k^4 + 2k^3 - 2k^2 - 3k - 3)}{(2k-3)(2k+1)(2k+5)},
\]

\[
a_{k,k+2} = a_{k+2,k} = -\frac{(k+1)(k+2)(2k+3)}{2(2k+5)(2k+1)},
\]

\[
a_{k,k+4} = a_{k+4,k} = \frac{(k+1)(k+2)(k+3)(k+4)}{2(2k+1)(2k+5)(2k+9)}.
\] (2.14)

Assume that \( \partial^2_x R_k(x) = \sum_{j=0}^{\infty} c_{kj} R_j(x) \). Then with the help of (2.9) and integration by parts, we obtain

\[
c_{kj} = \frac{(\partial^2_x R_k, R_j)}{(R_j, R_j)} = -\frac{(\partial_x R_k, \partial_x R_j)}{(R_j, R_j)} = -\frac{2j+1}{2} (\partial_x R_k, \partial_x R_j).
\] (2.15)

This, along with (2.14), leads to the result (2.11). In the same manner, we derive the result (2.12). \( \square \)

## 3 Diagonalized Legendre rational spectral methods

In this section, we propose a diagonalized Legendre rational spectral method for solving various differential equations.

### 3.1 Second-order problems

Consider the second order elliptic boundary value problem:

\[
\begin{cases}
-\partial^2_x u(x) + \mu u(x) = f(x), & \mu \geq 0, \ x \in \Lambda, \\
\lim_{|x| \to \infty} u(x) = 0.
\end{cases}
\] (3.1)

A weak formulation of (3.1) is to find \( u \in H^1(\Lambda) \) such that

\[
A_\mu(u,v) := (\partial_x u, \partial_x v) + \mu (u,v) = (f,v), \quad \forall v \in H^1(\Lambda).
\] (3.2)

Clearly, if \( f \in (H^1(\Lambda))' \), then by Lax-Milgram lemma, (3.2) admits a unique solution.

Next, let \( N \) be any positive integer, and \( \mathcal{R}_N(\Lambda) = \text{span} \{ R_0(x), R_1(x), \ldots, R_N(x) \} \). The Legendre rational spectral scheme for (3.2) is to find \( u_N \in \mathcal{R}_N(\Lambda) \) such that

\[
A_\mu(u_N, \phi) = (f,\phi), \quad \forall \phi \in \mathcal{R}_N(\Lambda).
\] (3.3)

To propose a diagonalized approximation scheme for (3.3), we need to construct new basis functions \( \{ \varphi_k \}_{0 \leq k \leq N} \), which are mutually orthogonal with respect to the Sobolev inner produce \( A_\mu(\cdot,\cdot) \).
Lemma 3.1. Let \( \varphi_k \in \mathcal{R}_k(\Lambda) \) be the Sobolev orthogonal Legendre rational function such that \( \varphi_k - R_k \in \mathcal{R}_{k-1}(\Lambda) \) and
\[
A_\mu(\varphi_k, \varphi_l) = \eta_k \delta_{k,l}, \quad k, l \geq 0.
\] (3.4)

Then we have
\[
\varphi_k(x) = R_k(x) - d_{k,1} \varphi_{k-2}(x) - d_{k,2} \varphi_{k-4}(x), \quad k \geq 0,
\] (3.5)
where \( \varphi_k(x) \equiv 0 \) \((k < 0)\), \( \eta_0 = 0 \) \((k < 0)\), \( d_{k,1} = 0 \) \((k < 2)\), \( d_{k,2} = 0 \) \((k < 4)\), and
\[
\eta_k = \frac{3(k^4 + 2k^3 - 2k^2 - 3k - 3)}{(2k+5)(2k-3)(2k+1)} + \frac{2\mu}{2k+1} - (d_{k,1})^2 \eta_{k-2} - (d_{k,2})^2 \eta_{k-4}, \quad k \geq 0,
\]
\[
d_{k,1} = -\frac{k(k-1)(2k-1)}{2(2k-3)(2k+1)} \eta_{k-2} - \frac{k(k-1)(k-2)(k-3)d_{k-2,1}}{2(2k-7)(2k-3)(2k+1)} \eta_{k-2}, \quad k \geq 2,
\]
\[
d_{k,2} = \frac{k(k-1)(k-2)(k-3)}{2(2k-7)(2k-3)(2k+1)} \eta_{k-4}, \quad k \geq 4. \] (3.6)

Proof. We first use mathematical induction to verify the result (3.5). According to the orthogonality assumption (3.4), we have
\[
\varphi_k(x) = R_k(x) - \sum_{l=0}^{k-1} \frac{A_\mu(R_k, \varphi_l)}{\eta_l} \varphi_l(x), \quad k \geq 1.
\] (3.7)

Due to the orthogonality (2.9), we know
\[
(R_k, \varphi) = 0, \quad \forall \varphi \in \mathcal{R}_{k-1}(\Lambda).
\] (3.8)

Therefore, with the help of (2.11), we obtain that
\[
A_\mu(R_1, \varphi_0) = (\partial_x R_1, \partial_x \varphi_0) = - (\partial_x^2 R_1, R_0) = 0.
\]

This means \( \varphi_1(x) = R_1(x) \). Similarly,
\[
A_\mu(R_2, \varphi_0) = (\partial_x R_2, \partial_x \varphi_0) + \mu(R_2, \varphi_0) = - (\partial_x^2 R_2, R_0) = - \frac{3}{\eta_0},
\]
\[
A_\mu(R_2, \varphi_1) = (\partial_x R_2, \partial_x \varphi_1) + \mu(R_2, \varphi_1) = - (\partial_x^2 R_2, R_1) = 0,
\]
which means \( \varphi_2(x) = R_2(x) - d_{2,1} \varphi_0(x) \) with the constant \( d_{2,1} = - \frac{3}{\eta_0} \). In the same manner, we can verify the results of (3.5) for \( k = 3,4 \), with the constants \( d_{3,1} = - \frac{5}{\eta_1}, d_{4,1} = - \frac{14+4d_{2,1}}{15\eta_2} \)
and \( d_{4,2} = \frac{1}{\eta_0} \) as in (3.6).

Next, assume that for any \( 0 \leq l \leq k-1 \) and \( k \geq 5 \),
\[
\varphi_l(x) = R_l(x) - d_{l,1} \varphi_{l-2}(x) - d_{l,2} \varphi_{l-4}(x).
\]
We shall prove that for \( k \geq 5 \),
\[
\varphi_k(x) = R_k(x) - d_{k,1} \varphi_{k-2}(x) - d_{k,2} \varphi_{k-4}(x).
\]
(3.9)

In fact, by (3.2), (3.8), (2.11) and the induction assumption, we derive that for \( k > l \geq 0 \) and \( k \geq 5 \),
\[
A_\mu(R_k, q_l) = (\partial_x R_k, \partial_x q_l) \]
\[
= (\partial_x R_k, \partial_x R_l) - d_{l,1}(\partial_x R_k, \partial_x q_{l-2}) - d_{l,2}(\partial_x R_k, \partial_x q_{l-4})
\]
\[
= (\partial_x R_k, \partial_x R_l) - d_{l,1}(\partial_x R_k, \partial_x R_{l-2}) + (d_{l,1}d_{l-2,1} - d_{l,2})(\partial_x R_k, \partial_x q_{l-4}) + d_{l,1}d_{l-2,2}(\partial_x R_k, \partial_x q_{l-6})
\]
\[
= -\left(\frac{k(k-1)(2k-1)}{2(2k-3)(2k+1)} + \frac{k(k-1)(k-2)(k-3)d_{k-2,1}}{2(2k-3)(2k-3)(2k+1)}\right)\delta_{k,l+2} + \frac{k(k-1)(k-2)(k-3)}{2(2k-3)(2k-3)(2k+1)}\delta_{k,l+4}.
\]

Hence, by (3.7) we verify the result (3.5) with
\[
d_{k,1} = -\frac{k(k-1)(2k-1)}{2(2k-3)(2k+1)\eta_{k-2}} - \frac{k(k-1)(k-2)(k-3)d_{k-2,1}}{2(2k-3)(2k-3)(2k+1)\eta_{k-2}},
\]
\[
d_{k,2} = \frac{k(k-1)(k-2)(k-3)}{2(2k-3)(2k-3)(2k+1)\eta_{k-4}}.
\]

It remains to confirm the constant \( \eta_k \). Clearly, by (2.9) and (2.11) we get
\[
A_\mu(R_k, R_k) = (\partial_x R_k, \partial_x R_k) + \mu(R_k, R_k) = \frac{3(k^4 + 2k^3 - 2k^2 - 3k - 3)}{(2k+5)(2k-3)(2k+1)} + \frac{2\mu}{2k+1}.
\]

On the other hand, by (3.5) we have
\[
A_\mu(R_k, R_k) = A_\mu(\varphi_k + d_{k,1} \varphi_{k-2} + d_{k,2} \varphi_{k-4}, \varphi_k + d_{k,1} \varphi_{k-2} + d_{k,2} \varphi_{k-4})
\]
\[
= \eta_k + (d_{k,1})^2 \eta_{k-2} + (d_{k,2})^2 \eta_{k-4}.
\]

Thereby
\[
\eta_k = \frac{3(k^4 + 2k^3 - 2k^2 - 3k - 3)}{(2k+5)(2k-3)(2k+1)} + \frac{2\mu}{2k+1} - (d_{k,1})^2 \eta_{k-2} - (d_{k,2})^2 \eta_{k-4}.
\]

This ends the proof. \( \square \)

Obviously, \( \mathcal{R}_N(\Lambda) = \{ \varphi_k(x) : 0 \leq k \leq N \} \). Thus the variational forms (3.2) and (3.3) together with the orthogonality of \( \{ \varphi_k(x) \} \) lead to the following main theorem in this subsection.

**Theorem 3.1.** Let \( u(x) \) and \( u_N(x) \) be the solution of (3.1) and (3.3), respectively. Then both \( u(x) \) and \( u_N(x) \) have the explicit representations in \( \{ \varphi_k(x) \} \),
\[
u(x) = \sum_{k=0}^\infty \hat{u}_k \varphi_k(x), \quad u_N(x) = \sum_{k=0}^N \hat{u}_k \varphi_k(x),
\]
\[
\hat{u}_k = \frac{1}{\eta_k} A_\mu(u, \varphi_k) = \frac{1}{\eta_k} (f, \varphi_k), \quad k \geq 0.
\]
3.2 Fourth-order problems

Consider the fourth order elliptic boundary value problem:

$$\begin{cases}
\partial^4_x u(x) - a \partial^2_x u(x) + \beta u(x) = f(x), & \alpha, \beta \geq 0, \ x \in \Lambda, \\
\lim_{|x| \to \infty} u(x) = \lim_{|x| \to \infty} \partial_x u(x) = 0.
\end{cases}$$

(3.10)

A weak formulation of (3.10) is to find $u \in H^2(\Lambda)$ such that

$$B_{\alpha, \beta}(u, v) := (\partial^2_x u, \partial^2_x v) + \alpha (\partial_x u, \partial_x v) + \beta (u, v) = (f, v), \quad \forall v \in H^2(\Lambda).$$

(3.11)

Clearly, if $f \in (H^2(\Lambda))^\prime$, then by Lax-Milgram lemma, (3.11) admits a unique solution.

The Legendre rational spectral scheme for (3.11) is to find

$$u \in H^2(\Lambda).$$

To propose a diagonalized approximation scheme for (3.12), we need to construct new basis functions $\{\psi_k\}_{0 \leq k \leq N}$, which are mutually orthogonal with respect to the Sobolev inner product $B_{\alpha, \beta}(\cdot, \cdot)$.

**Lemma 3.2.** Let $\psi_k \in \mathcal{R}_k(\Lambda)$ be the Sobolev orthogonal Legendre rational functions such that

$$\psi_k - R_k \in \mathcal{R}_{k-1}(\Lambda)$$

and

$$B_{\alpha, \beta}(\psi_k, \psi_l) = \sigma_k \delta_{k,l}, \quad k, l \geq 0.$$  

(3.13)

Then the following recurrence relation holds:

$$\psi_k(x) = R_k(x) - a_k \psi_{k-2}(x) - b_k \psi_{k-4}(x) - c_k \psi_{k-6}(x) - d_k \psi_{k-8}(x), \quad k \geq 0,$$

(3.14)

where $\psi_k(x) \equiv 0 \ (k < 0)$, $\sigma_k = 0 \ (k < 0)$, $a_k = 0 \ (k < 2)$, $b_k = 0 \ (k < 4)$, $c_k = 0 \ (k < 6)$, $d_k = 0 \ (k < 8)$, and

(i). $\sigma_k = -(a_k)^2 \sigma_{k-2} - (b_k)^2 \sigma_{k-4} - (c_k)^2 \sigma_{k-6} - (d_k)^2 \sigma_{k-8} + \frac{35k^8 + 140k^7 - 310k^6 - 1420k^5 - 2542k^4 - 2554k^3 + 6921k^2 + 7938k + 5292}{4(2k+9)(2k+5)(2k+1)(2k-3)(2k-7)}$

$$+ \alpha \frac{3(k^4 + 2k^3 - 2k^2 - 3k - 3)}{(2k+5)(2k-3)(2k+1)} + \frac{2\beta}{2k+1}, \quad k \geq 0,$$
(ii). For $k < 2, a_k = -\frac{k(k-1)(14k^5 - 35k^4 - 48k^3 + 107k^2 - 446k + 204)}{4(2k+5)(2k+1)(2k-3)(2k-7)\sigma_{k-2}}$

$\quad -a_{k-2}\frac{k(k-1)(k-2)(k-3)(28k^4 - 168k^3 - 32k^2 + 852k - 1391)}{8(2k+5)(2k+1)(2k-3)(2k-7)(2k-11)\sigma_{k-2}}$

$\quad - (a_{k-2} - b_{k-2})\frac{k(k-1)(k-2)(k-3)(k-4)(k-5)(2k-5)}{4(2k+1)(2k-3)(2k-7)(2k-11)\sigma_{k-2}}$

$\quad + (a_{k-2}b_{k-4} - c_{k-2} - (a_{k-2}a_{k-4} - b_{k-2}a_{k-6})$

$\times \frac{k(k-1)(k-2)(k-3)(k-4)(k-5)(k-6)(k-7)}{8(2k+1)(2k-3)(2k-7)(2k-11)(2k-15)\sigma_{k-2}}$

$\quad - a\left(\frac{k(k-1)(2k-1)}{2(2k-3)(2k+1)\sigma_{k-2}} + a_{k-2}\frac{k(k-1)(k-2)(k-3)}{2(2k-7)(2k-3)(2k+1)\sigma_{k-2}}\right),$

(iii). For $k < 4, b_k = \frac{k(k-1)(k-2)(k-3)(28k^4 - 168k^3 - 32k^2 + 852k - 1391)}{8(2k+5)(2k+1)(2k-3)(2k-7)(2k-11)\sigma_{k-4}}$

$\quad + a_{k-4}\frac{k(k-1)(k-2)(k-3)(k-4)(k-5)(2k-5)}{4(2k+1)(2k-3)(2k-7)(2k-11)\sigma_{k-4}}$

$\quad + (a_{k-4}a_{k-6} - b_{k-4})\frac{k(k-1)(k-2)(k-3)(k-4)(k-5)(k-6)(k-7)}{8(2k+1)(2k-3)(2k-7)(2k-11)(2k-15)\sigma_{k-4}}$

$\quad + a\frac{k(k-1)(k-2)(k-3)}{2(2k-7)(2k-3)(2k+1)\sigma_{k-4}},$

(iv). For $k < 6, c_k = -\frac{k(k-1)(k-2)(k-3)(k-4)(k-5)(2k-5)}{4(2k+1)(2k-3)(2k-7)(2k-11)\sigma_{k-6}}$

$\quad - a_{k-6}\frac{k(k-1)(k-2)(k-3)(k-4)(k-5)(k-6)(k-7)}{8(2k+1)(2k-3)(2k-7)(2k-11)(2k-15)\sigma_{k-6}},$

(v). For $k < 8, d_k = \frac{k(k-1)(k-2)(k-3)(k-4)(k-5)(k-6)(k-7)}{8(2k+1)(2k-3)(2k-7)(2k-11)(2k-15)\sigma_{k-8}}.$

Proof. According to the orthogonality assumption (3.13), we have

$$\psi_k(x) = R_k(x) - \sum_{m=0}^{k-1} \frac{B_{a,\beta}(R_k,\psi_m)}{\sigma_m} \psi_m(x), \quad k \geq 1.$$ (3.15)
We first use mathematical induction to verify (3.14). By (2.9) we have \( (R_k, \psi_m) = 0, \forall m < k \). Therefore, by (2.11) and (2.12) we obtain

\[
B_{a,\beta}(R_1, \psi_0) = (\partial_x^2 R_1, \partial_x^2 \psi_0) + a(\partial_x R_1, \partial_x \psi_0) = (\partial_x^4 R_1, R_0) - a(\partial_x^2 R_1, R_0) = 0.
\]

Thus, \( \psi_1(x) = R_1(x) \). Similarly,

\[
B_{a,\beta}(R_2, \psi_0) = (\partial_x^2 R_2, \partial_x^2 \psi_0) + a(\partial_x R_2, \partial_x \psi_0) = (\partial_x^4 R_2, R_0) - a(\partial_x^2 R_2, R_0) = -\frac{14+3\alpha}{8},
\]

\[
B_{a,\beta}(R_2, \psi_1) = (\partial_x^2 R_2, \partial_x^2 \psi_1) + a(\partial_x R_2, \partial_x \psi_1) = (\partial_x^4 R_2, R_1) - a(\partial_x^2 R_2, R_1) = 0,
\]

which means \( \psi_2(x) = R_2(x) - a_2 \psi_0(x) \) with the constant \( a_2 = -\frac{14+3\alpha}{8n_0} \). In the same manner, we can verify the results of (3.14) for \( k \leq 8 \).

Next, assume that for any \( 0 \leq l \leq k-1 \) and \( k \geq 9 \),

\[
\psi_l(x) = R_l(x) - a_l \psi_{l-2}(x) - b_l \psi_{l-4}(x) - c_l \psi_{l-6}(x) - d_l \psi_{l-8}(x).
\]

We shall prove that for \( k \geq 9 \),

\[
\psi_k(x) = R_k(x) - a_k \psi_{k-2}(x) - b_k \psi_{k-4}(x) - c_k \psi_{k-6}(x) - d_k \psi_{k-8}(x).
\]

In fact, by (2.9) and (3.11), we deduce that for any \( k > m \geq 0 \),

\[
B_{a,\beta}(R_k, \psi_m) = (\partial_x^2 R_k, \partial_x^2 \psi_m) + a(\partial_x R_k, \partial_x \psi_m) = (\partial_x^4 R_k, \psi_m) - a(\partial_x^2 R_k, \psi_m).
\]  

(3.16)

From (2.11), (2.12) and (2.9), we know that \( (\partial_x^4 R_k, \psi_m) = (\partial_x^2 R_k, \psi_m) = 0 \) for \( 0 \leq m \leq k-9 \) and \( 0 \leq n \leq k-5 \). Therefore, by (3.15) we get

\[
R_k(x) = \psi_k(x) + a_k \psi_{k-2}(x) + b_k \psi_{k-4}(x) + c_k \psi_{k-6}(x) + d_k \psi_{k-8}(x), \quad k \geq 9.
\]

Next, by (2.11), (2.12), (2.9), (3.13) and the induction assumption, we know that for \( k \geq 9 \),

\[
B_{a,\beta}(R_k, \psi_k-1) = (\partial_x^2 R_k, \partial_x^2 \psi_{k-1}) + a(\partial_x R_k, \partial_x \psi_{k-1}) = (\partial_x^4 R_k, \psi_{k-1}) - a(\partial_x^2 R_k, \psi_{k-1})
\]

\[
= (\partial_x^4 R_k - a\partial_x^2 R_k, R_{k-1} - a_{k-1} \psi_{k-3} - b_{k-1} \psi_{k-5} - c_{k-1} \psi_{k-7} - d_{k-1} \psi_{k-9})
\]

\[
= 0.
\]

On the other hand,

\[
B_{a,\beta}(R_k, \psi_k-1) = B_{a,\beta}(\psi_k + a_k \psi_{k-2} + b_k \psi_{k-4} + c_k \psi_{k-6} + d_k \psi_{k-8}, \psi_{k-1}) = a_k \sigma_{k-1}.
\]

Hence, \( a_k = 0 \). Similarly, we have \( b_k = c_k = d_k = 0 \). This leads to the result (3.14).
It remains to confirm the coefficients \( a_k, b_k, c_k, d_k \) and \( \sigma_k \). Actually, by using (2.11), (2.12) and (2.9), we obtain that for \( k > m \geq 0 \) and \( k \geq 9 \),

\[
B_{a, \beta}(R_k, \psi_m) = B_{a, \beta}(\psi_k + a_k \psi_{k-2} + b_k \psi_{k-4} + c_k \psi_{k-6} + d_k \psi_{k-8}, \psi_m). \tag{3.17}
\]

On the other hand,

\[
B_{a, \beta}(R_k, \psi_m) = (\partial^4_x R_k, \psi_m) - \alpha (\partial^2_x R_k, \psi_m) = (\partial^4_x R_k - \alpha \partial^2_x R_k, R_m - a_m \psi_{m-2} - b_m \psi_{m-4} - c_m \psi_{m-6} - d_m \psi_{m-8}) \]

\[
= (\partial^4_x R_k - \alpha \partial^2_x R_k, R_m - a_m R_{m-2} + (a_m a_{m-2} - b_m) R_{m-4} + (a_m b_{m-2} - a_m a_{m-2} a_{m-4} + b_m a_{m-4} - c_m) R_{m-6}). \tag{3.18}
\]

Taking \( m = k - 2, k - 4, k - 6, k - 8 \) in (3.17) and (3.18) respectively, we derive the results (ii)-(v) in Lemma 3.2.

We next confirm the constant \( \sigma_k \). By using (2.11), (2.12), (2.9) and (3.13), we know that for \( k \geq 9 \),

\[
B_{a, \beta}(R_k, R_k) = (\partial^4_x R_k, R_k) - \alpha (\partial^2_x R_k, R_k) + \beta (R_k, R_k),
\]

\[
= \frac{35k^6 + 140k^7 - 310k^6 - 1420k^5 - 2542k^4 - 2554k^3 + 6921k^2 + 7938k + 5292}{4(2k + 9)(2k + 5)(2k + 1)(2k - 3)(2k - 7)}
\]

\[
+ \frac{3\alpha (k^4 + k^3 - 2k^2 - 3k - 3)}{(2k + 5)(2k - 3)(2k + 1)} + \frac{2\beta}{2k + 1},
\]

and

\[
B_{a, \beta}(R_k, R_k) = B_{a, \beta}(\psi_k + a_k \psi_{k-2} + b_k \psi_{k-4} + c_k \psi_{k-6} + d_k \psi_{k-8},
\]

\[
\psi_k + a_k \psi_{k-2} + b_k \psi_{k-4} + c_k \psi_{k-6} + d_k \psi_{k-8})
\]

\[
= \sigma_k + (a_k)^2 \sigma_{k-2} + (b_k)^2 \sigma_{k-4} + (c_k)^2 \sigma_{k-6} + (d_k)^2 \sigma_{k-8}.
\]

This gives the result (i) of Lemma 3.2. \( \square \)

**Theorem 3.2.** Let \( u(x) \) and \( u_N(x) \) be the solution of (3.10) and (3.12), respectively. Then both \( u(x) \) and \( u_N(x) \) have the explicit representations in \( \{ \psi_k(x) \} \),

\[
u(x) = \sum_{k=0}^{\infty} \hat{u}_k \psi_k(x), \quad u_N(x) = \sum_{k=0}^{N} \hat{u}_k \psi_k(x),
\]

\[
\hat{u}_k = \frac{1}{\sigma_k} B_{a, \beta}(u, \psi_k) = \frac{1}{\sigma_k} (f, \psi_k), \quad k \geq 0.
\]
3.3 The nonlinear heat equation

Consider the following nonlinear heat equation,

\[
\begin{aligned}
&\partial_t u(x,t) - \partial_x^2 u(x,t) + \mu u(x,t) + u^2(x,t) = f(x,t), \quad x \in \Lambda, \quad t \in (0, T], \\
&\lim_{|x| \to \infty} u(x,t) = 0, \quad t \in [0, T], \\
&u(x,0) = u_0(x), \quad x \in \Lambda,
\end{aligned}
\]  

(3.19)

where \( \mu > 0 \) and \( f(x,t) \) is a given function.

We shall propose an efficient spectral-finite difference scheme based on diagonalized Legendre rational spectral method in space and the finite difference method in time.

Denote by \( \tau \) the time step size, \( M = [\frac{T}{\tau}] \), and \( u^{(k)}(x) = u(x,k\tau), \ k = 0, 1, \ldots, M \). Then, a standard centered difference scheme in time is given by

\[
\begin{aligned}
&\left\{ \begin{array}{l}
\frac{u^{(k+1)}(x) - u^{(k)}(x)}{\tau} \ - \partial_x^2 u^{(k+1)}(x) + \partial_x^2 u^{(k)}(x) + \mu u^{(k+1)}(x) + u^{(k)}(x) \\
\quad + \frac{(u^{(k+1)}(x))^2 + (u^{(k)}(x))^2}{2} = \frac{f^{(k+1)}(x) + f^{(k)}(x)}{2}, \\
\quad \lim_{|x| \to \infty} u^{(k)}(x) = 0, \quad k = 0, 1, \ldots, M, \\
u^{(0)}(x) = u_0(x), \quad x \in \Lambda.
\end{array} \right.
\]  

(3.20)

A weak formulation of (3.20) is to find \( u^{(k+1)}(x) \in H^1(\Lambda) \) such that

\[
A_{\tau,\mu}(u^{(k+1)}, v) := \tau (\partial_x u^{(k+1)}, \partial_x v) + (2 + \tau \mu)(u^{(k+1)}, v) = (g^{(k)}, v), \quad \forall v \in H^1(\Lambda),
\]  

(3.21)

where

\[
g^{(k)}(x) = \tau f^{(k+1)}(x) + \tau f^{(k)}(x) + \tau \partial_x^2 u^{(k)}(x) + (2 - \tau \mu) u^{(k)}(x) - \tau (u^{(k+1)}(x))^2 - \tau (u^{(k)}(x))^2.
\]

The Legendre rational spectral scheme for (3.21) is to find \( u_N^{(k+1)} \in R_N(\Lambda) \) such that

\[
A_{\tau,\mu}(u_N^{(k+1)}, \phi) = (g_N^{(k)}, \phi), \quad \forall \phi \in R_N(\Lambda),
\]  

(3.22)

where

\[
g_N^{(k)}(x) = \tau f^{(k+1)}(x) + \tau f^{(k)}(x) + \tau \partial_x^2 u_N^{(k)}(x) + (2 - \tau \mu) u_N^{(k)}(x) - \tau (u_N^{(k+1)}(x))^2 - \tau (u_N^{(k)}(x))^2.
\]

To propose a diagonalized Legendre rational spectral scheme for (3.22), we need to construct new basis functions \( \{ \Psi_k(x) \}_{0 \leq k \leq N} \), which are mutually orthogonal with respect to the Sobolev inner product \( A_{\tau,\mu}(\cdot, \cdot) \).
**Lemma 3.3.** Let $\Psi_k \in \mathcal{R}_k(\Lambda)$ be the Sobolev orthogonal Legendre rational functions such that $\Psi_k - R_k \in \mathcal{R}_{k-1}(\Lambda)$ and

$$A_{p,m}(\Psi_k, \Psi_I) = \gamma_k \delta_{k,l}, \quad k, l \geq 0. \tag{3.23}$$

Then we have

$$\Psi_k(x) = R_k(x) - d_{k,1} \Psi_{k-2}(x) - d_{k,2} \Psi_{k-4}(x), \quad k \geq 0, \tag{3.24}$$

where $\Psi_k(x) \equiv 0 \ (k < 0)$, $\gamma_k = 0 \ (k < 0)$, $d_{k,1} = 0 \ (k < 2)$, $d_{k,2} = 0 \ (k < 4)$, and

$$\gamma_k = \frac{3 \tau (k^4 + 2k^3 - 2k^2 - 3k - 3)}{(2k+5)(2k-3)(2k+1)} + \frac{4 + 2 \tau \mu}{2k+1} - (d_{k,1})^2 \gamma_{k-2} - (d_{k,2})^2 \gamma_{k-4}, \quad k \geq 0,$$

$$d_{k,1} = -\frac{\tau k (k-1)(2k-1)}{2(2k-3)(2k+1) \gamma_{k-2}} - \frac{\tau k (k-1)(2k-3) d_{k-2,1}}{2(2k-7)(2k-3)(2k+1) \gamma_{k-2}}, \quad k \geq 2,$$

$$d_{k,2} = \frac{\tau k (k-1)(2k-3) d_{k-2,1}}{2(2k-7)(2k-3)(2k+1) \gamma_{k-4}}, \quad k \geq 4.$$

**Proof.** The proof is in the same way as Lemma 3.1. We neglect the details. \qed

**Theorem 3.3.** Let $u_N^{(k+1)}(x)$ be the solution of (3.22). Then we have

$$u_N^{(k+1)}(x) = \sum_{l=0}^{N} \hat{u}_l^{(k+1)} \Psi_l(x), \quad \hat{u}_l^{(k+1)} = \frac{1}{\gamma_l} \langle \delta_N^{(k)}, \Psi_l \rangle, \quad l \geq 0.$$

**Remark 3.1.** This is an implicit scheme. In actual computation, an iterative process should be employed to evaluate the expansion coefficients.

### 4 Numerical results

In this section, we examine the effectiveness and the accuracy of the diagonalized Legendre rational spectral method for solving elliptic equations and nonlinear heat equation.

We first examine the second order problem (3.1) with $\mu = 1$, and consider the following two cases of the smooth solutions with different decay properties.

- $u(x) = e^{-x^2} \sin(kx)$, which is exponential decay with oscillation. In Figure 1, we plot the $\log_{10}$ of the discrete $L^2$- and $H^1$- errors vs. $N$ with $k = 2$. The two near straight lines indicate a geometric convergence rate.

- $u(x) = \frac{\sin(kx)}{(k^2 + 1)^{\mu}}$, which is algebraic decay with oscillation. In Figure 2, we plot the $\log_{10}$ of the discrete $L^2$- and $H^1$- errors vs. $N$ with $k = h = 2$. Clearly, an algebraic convergence rate is observed.
We next examine the fourth order problem (3.10) with $\alpha = \beta = 1$, and consider the following two cases of the smooth solutions with different decay properties.

- $u(x) = e^{-x^2} \sin(kx)$, which is exponential decay with oscillation. In Figure 3, we plot the $\log_{10}$ of the discrete $L^2$- and $H^1$-errors vs. $N$ with $k = 2$. Again, a geometric convergence rate is observed.

- $u(x) = \frac{1}{(x^2+1)^h}$, which is algebraic decay. In Figure 4, we plot the $\log_{10}$ of the discrete $L^2$- and $H^1$-errors vs. $N$ with $h = 2, 3, 4, 5, 6$. The near straight lines indicate an algebraic convergence rate. They also show that the faster the exact solution decays, the smaller the numerical errors would be.

We finally consider the nonlinear heat equation (3.19) with $\mu = 1$, and consider the following two cases of the smooth solutions with different decay properties.
• \( u(x,t) = e^{-x^2} \sin(k_1 x + k_2 t) \), which is exponential decay with oscillation. In Figures 5 and 6, we plot the log_{10} of the discrete \( L^2 \)- and \( H^1 \)-errors vs. \( N \) with \( \tau = 0.1, 0.01, 0.001, 0.0001 \) and \( k_1 = 2, k_2 = 1 \), respectively. Clearly, a geometric convergence rate is observed. They also indicate that the smaller the time step size \( \tau \), the smaller the numerical errors would be. In Figure 7, we plot the values of \( L^2 \)-errors for \( 0 \leq t \leq 100 \) with \( \tau = 0.01 \). It demonstrates the stability of long-time calculation of scheme (3.21).

• \( u(x,t) = \frac{\sin(k_1 x + k_2 t)}{(x^2+1)^h} \), which is algebraic decay with oscillation. In Figure 8, we plot the log_{10} of the discrete \( L^2 \)-errors vs. \( N \) with \( h = 2 \) and various \( \tau \). They indicate an algebraic convergence rate.

To demonstrate the essential superiority of the diagonalized Legendre rational spectral method to the classic Legendre rational and Hermite spectral methods, we also ex-
amine the issues on the condition numbers for the resulting algebraic systems and the computational cost.

The basis functions in the diagonalized Legendre rational spectral method are chosen as \( \{ \phi_k(x) \sqrt{\eta_k} \}_{k=0}^N \), \( \{ \psi_k(x) \sqrt{\sigma_k} \}_{k=0}^N \) and \( \{ \Psi_k(x) \sqrt{\gamma_k} \}_{k=0}^N \), which are Sobolev orthogonal. Accordingly, the condition numbers are equal to 1.

For the classical Legendre rational and Hermite spectral methods, the basis functions are chosen as \( \{ R_k(x) \}_{k=0}^N \) or \( \{ H_k(x) := (-1)^k \frac{e^{x^2} \partial_k (e^{-x^2})}{2^k k!} \}_{k=0}^N \). The corresponding stiffness matrices have off-diagonal entries. In Tables 1 and 2 below, we list the condition numbers of the classical Legendre rational spectral method and Hermite spectral method for (3.1) and (3.10). Note that the condition numbers in Table 1 increase as \( O(N^2) \) for the second order problem (3.1) and \( O(N^4) \) for the fourth order problem (3.10) by the classical Legendre rational spectral method with \( \alpha = \beta = \mu = 1 \). Moreover, the condition numbers in Table 2 increase as \( O(N) \) for the second order problem (3.1) and \( O(N^2) \) for the fourth order problem (3.10) by the Hermite spectral method with \( \alpha = \beta = \mu = 1 \).

For comparison of the computational cost between the diagonalized Legendre rational spectral method and the classical Legendre rational spectral method, we consider the problem (3.10) with \( \alpha = \beta = 1 \). In Tables 3 and 4, we list the \( L^2 \)-errors and the corresponding computational cost. It can be observed that our diagonalized spectral method costs much less CPU time.

### Table 1: Condition numbers of the classical Legendre rational spectral method.

<table>
<thead>
<tr>
<th>Method</th>
<th>N = 60</th>
<th>N = 120</th>
<th>N = 180</th>
<th>N = 240</th>
<th>N = 300</th>
<th>N = 360</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eq. (3.1)</td>
<td>1.6805e+3</td>
<td>8.1815e+3</td>
<td>2.0169e+4</td>
<td>3.7915e+4</td>
<td>6.1581e+4</td>
<td>9.1282e+4</td>
</tr>
<tr>
<td>Eq. (3.10)</td>
<td>3.7874e+6</td>
<td>8.5563e+7</td>
<td>5.0665e+8</td>
<td>1.7595e+9</td>
<td>4.5824e+9</td>
<td>9.9674e+9</td>
</tr>
</tbody>
</table>

### Table 2: Condition numbers of Hermite spectral method.

<table>
<thead>
<tr>
<th>Method</th>
<th>N = 30</th>
<th>N = 60</th>
<th>N = 90</th>
<th>N = 120</th>
<th>N = 150</th>
<th>N = 180</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eq. (3.1)</td>
<td>4.7998e+1</td>
<td>1.0398e+2</td>
<td>1.6122e+2</td>
<td>2.1904e+2</td>
<td>2.7721e+2</td>
<td>3.3562e+2</td>
</tr>
<tr>
<td>Eq. (3.10)</td>
<td>2.3738e+3</td>
<td>1.1001e+4</td>
<td>2.6311e+4</td>
<td>4.8434e+4</td>
<td>7.7440e+4</td>
<td>1.1337e+5</td>
</tr>
</tbody>
</table>

### Table 3: Diagonalized Legendre rational spectral method for (3.10).

<table>
<thead>
<tr>
<th>L2 Errors</th>
<th>N = 50</th>
<th>N = 100</th>
<th>N = 150</th>
<th>N = 200</th>
<th>N = 250</th>
<th>N = 300</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU time</td>
<td>0.2242</td>
<td>0.2295</td>
<td>0.2370</td>
<td>0.2463</td>
<td>0.2581</td>
<td>0.2711</td>
</tr>
</tbody>
</table>

### Table 4: Classical Legendre rational spectral method for (3.10).

<table>
<thead>
<tr>
<th>L2 Errors</th>
<th>N = 50</th>
<th>N = 100</th>
<th>N = 150</th>
<th>N = 200</th>
<th>N = 250</th>
<th>N = 300</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU time</td>
<td>1.9761</td>
<td>1.9770</td>
<td>1.9786</td>
<td>1.9808</td>
<td>1.9843</td>
<td>1.9872</td>
</tr>
</tbody>
</table>
Acknowledgments

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References