Research Article

Linear Barycentric Rational Method for Solving Schrodinger Equation

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A linear barycentric rational collocation method (LBRCM) for solving Schrodinger equation (SDE) is proposed. According to the barycentric interpolation method (BIM) of rational polynomial and Chebyshev polynomial, the matrix form of the collocation method (CM) that is easy to program is obtained. The convergence rate of the LBRCM for solving the Schrodinger equation is proved from the convergence rate of linear barycentric rational interpolation. Finally, a numerical example verifies the correctness of the theoretical analysis.

1. Introduction

Schrodinger equation (SDE) is widely used in atomic physics, nuclear physics and solid physics, quantum mechanics, and so on. SDE is only applicable to nonrelativistic particles with low velocity, and there is no description of particle spin. In this paper, we are concerned with solving the numerical solution of the SDE:

$$ih\frac{\partial \phi(x, t)}{\partial t} = \frac{\hbar^2}{2m} \frac{\partial^2 \phi(x, t)}{\partial x^2} + V(x, t)\phi(x, t) + f(x, t),$$

(1)

$$\phi(x, 0) = g_1(x), \phi(x, t) = g_2(x), x \in (a, b),$$

(2)

$$\phi(a, t) = h_1(t), \phi(b, t) = h_2(t), \; \; 0 < t < T,$$

(3)

where $h$ is reduced Planck constant and $m$ denotes quality. In [1], the fractional Schrodinger–Choquard equation with blow-up criteria and instability of normalized standing waves is studied. In [2], the finite-difference time-domain (FDTD) method is studied to solve SDE. In [3], nonlinear magnetic Schrodinger–Poisson type equation is studied. In [4], high-order multiscale discontinuous Galerkin method for one-dimensional stationary SDEs with oscillating solutions is presented. In [5], sixth-order nonlinear SDE is concerned by factorization formula and an analytical method. In [6], nonlinear SDEs are solved by the iterative method. In [7], the two-dimensional Klein–Gordon SDEs are solved by linear compact alternating direction implicit (CADI) scheme.

For getting the equidistant node of the barycentric formula, Floater [8–10] has proposed a reasonable interpolation method; in particular, equidistant distribution nodes and the quasi-equidistant nodes have high numerical stability and accuracy of interpolation [11, 12]. In [13, 14], the linear barycentric rational collocation method (LBRCM) have been used to solve the integro-differential equation. Wang et al. [15–17] have expanded the application fields of the collocation method (CM), such as initial value problems, plane elasticity problems, and nonlinear problems. LBRCM for solving heat conduction equation and biharmonic equation are studied in [18, 19].

In this paper, a LBRCM for solving SDE is proposed. According to the barycentric interpolation method (BIM) of rational polynomial and Chebyshev polynomial, the matrix form of the collocation method that is easy to program is obtained. The convergence rate of the LBRC method for
solving the telegraph equation is proved from the convergence rate of linear barycentric rational interpolation (LBRI). Finally, a numerical example verifies the correctness of the theoretical analysis.

The remaining of this paper is planned as follows. Section 2 presents the differentiation matrices, CM for SDE, and the matrix form of CM. In Section 3, the convergence rate is proved. Finally, a numerical example verifies the theoretical analysis.

2. Differentiation Matrices of SDE

We partition the interval $[a, b]$ and $[0, T]$ into $a = x_0 < x_1 < \cdots < x_m = b$ and $0 = t_0 < t_1 < \cdots < t_n = T$ with $h_i = x_i - x_{i-1}$, $i = 0, 1, \ldots, m$, and $\tau_j = t_j - t_{j-1}$, $j = 0, 1, \ldots, n$, for the uniform partition with $h = (b - a)/m$ and $\tau = T/n$. For $\Omega = [a, b] \times [0, T]$ with $(x_i, t_j)$, $i = 0, 1, \ldots, m$ and $j = 0, 1, \ldots, n$ will be the uniform partition.

Consider the barycentric interpolation function (BIF) as

$$
\varphi(x_i, t) = \varphi(x_i), \quad i = 0, 1, \ldots, m,
$$

and its barycentric interpolation approximation is

$$
\varphi(x, t) = \sum_{i=0}^{m} \sum_{j=0}^{n} r_i(x) r_j(t) \varphi_{ij},
$$

where

$$
r_i(x) = \frac{w_i/(x - x_i)}{\sum_{k=0}^{n} w_k/(x - x_k)},
$$

and

$$
r_j(t) = \frac{w_j/(t - t_j)}{\sum_{k=0}^{n} w_k/(t - t_k)},
$$

where $f_i = \{ k \in I_m; i - d_i \leq k \leq i \}$, $I_m = \{ 0, \ldots, m - d_i \}$, and

$$
\varphi_{ij} = \left\{ \begin{array}{ll}
\varphi_i & \text{if } i \neq j,
- \varphi_i & \text{if } i = j.
\end{array} \right.
$$

Combining equations (1) and (5), we obtain

$$
i(I_m \otimes D^{(1)}) = (C^{(2)} \otimes I_m) - I_m \otimes f_m,
$$

and then, we have

$$
[I_m \otimes D^{(1)} + (C^{(2)} \otimes I_m) - I_m \otimes I_n] \Phi = F,
$$

where

$$
L = iI_m \otimes D^{(1)} + (C^{(2)} \otimes I_m) - I_m \otimes I_n,
$$

and

$$
D^{(1)}_{ij} = \begin{cases}
\frac{w_i/w_j}{x_i - x_j} & i \neq j, \\
- \sum_{k \neq i} D^{(1)}_{ik}, & i = j.
\end{cases}
$$

and

$$
C^{(1)}_{ij} = \begin{cases}
\frac{w_i/w_j}{x_i - x_j} & i \neq j, \\
- \sum_{k \neq i} C^{(1)}_{ik}, & i = j.
\end{cases}
$$

and

$$
C^{(2)}_{ij} = \begin{cases}
\frac{2C^{(1)}_{ij}(D^{(1)}_{ij} - \frac{1}{x_i - x_j})}{x_i - x_j}, & i \neq j, \\
- \sum_{k \neq i} C^{(2)}_{ik}, & i = j.
\end{cases}
$$

and $\otimes$ is Kronecker product of matrix. In the following, we define the Kronecher product of matrix $A = (a_{ij})_{m \times n}$ and $B = (b_{ij})_{k \times l}$ as

$$
A \otimes B = (a_{ij}B)_{m \times n \times k \times l},
$$

where

$$
a_{ij}B = \begin{bmatrix}
a_{i1}b_{11} & a_{i1}b_{12} & \cdots & a_{i1}b_{1l} \\
a_{i2}b_{21} & a_{i2}b_{22} & \cdots & a_{i2}b_{2l} \\
\vdots & \vdots & \ddots & \vdots \\
a_{in}b_{n1} & a_{in}b_{n2} & \cdots & a_{in}b_{nl}
\end{bmatrix}.
$$

3. Convergence Rate and Error Analysis

The barycentric rational interpolants of function (BIF) $\Phi(x)$ with $r(x)$ and its error convergence rate is

$$
e(x) := \varphi(x) - r_n(x) = (x - x_i) \cdots (x - x_{i-1}) (x - x_{i+d_x}) \varphi(x_i, x_{i+1}, \ldots, x_{i+d_x}, x),
$$

and

$$
e(x) = \sum_{i=0}^{n-d_x} \lambda_i(x) (\varphi(x) - r_n(x)) = A(x)/B(x) = O(h^{d_x+1}),
$$

where

$$
L \Phi = F,
$$
\[ A(x) := \sum_{i=0}^{n-d} (-1)^i \varphi[x_i, x_{i+1}, \ldots, x_{i+d}, x], \tag{18} \]

and

\[ B(x) = \sum_{i=0}^{n-d} \lambda_i(x), \tag{19} \]

where

\[ \lambda_i(x) = \frac{(-1)^i}{(x-x_i) \cdots (x-x_{i+d})} \tag{20} \]

The following Lemma was proved by Jean-Pau Berrut in [11].

\[ \omega_{ij} = \sum_{k_1 \in I_i} \sum_{k_2 \in I_j} (-1)^{i-d_1+j-d_2} \prod_{h_1=h_1(h_i k_i \neq j)} \frac{1}{x_i-x_{h}} \prod_{h_2=h_2(k_i k_2 \neq j)} \frac{1}{t_j-t_{h}} \tag{23} \]

and \( I_i = \{k_1 \in I_m: i-d_1 \leq k_1 \leq i\}, I_m = \{0, \ldots, m-d_1\}, \)

\[ I_j = \{k_2 \in I_m: j-d_2 \leq k_2 \leq j\}, I_n = \{0, \ldots, n-d_2\}. \tag{24} \]

By the error term of Newton–Cotes rule for two-dimensional function, we have

\[ e(x,t) := \varphi(x,t) - r(x,t) = \varphi(x,t) - r_n(x,t) \]

\[ = (x-x_i) \cdots (x-x_{i+d_i}) \varphi[x_i, x_{i+1}, \ldots, x_{i+d_i}, x] + (t-t_j) \cdots (t-t_{j+d_j}) \varphi[t_j, t_{j+1}, \ldots, t_{j+d_j}, t]. \tag{25} \]

**Lemma 1** (see [11]), For \( \varphi(x,t) \) defined in (16), we have

\[ \begin{align*}
|e(x,t)| & \leq C h^{d+1}, & \varphi & \in C^{d+2}[a,b], \\
|e'(x,t)| & \leq C h^{d}, & \varphi & \in C^{d+3}[a,b], \\
|e''(x,t)| & \leq C h^{d-1}, & \varphi & \in C^{d+4}[a,b], d \geq 1.
\end{align*} \tag{21} \]

For the BRIF \( \varphi(x,t) \) with \( r(x,t) \), we can get the bar-centric rational interpolation (BRI):

\[ r_n(x,t) = \frac{\sum_{i=0}^{m} \sum_{j=0}^{n} w_{ij}/[(x-x_i)(t-t_j)] \varphi_{ij}}{\sum_{i=0}^{m} \sum_{j=0}^{n} w_{ij}/(x-x_i)(t-t_j)}, \tag{22} \]

where

\[ \omega_{ij} = \sum_{k_1 \in I_i} \sum_{k_2 \in I_j} (-1)^{i-d_1+j-d_2} \prod_{h_1=h_1(h_i k_i \neq j)} \frac{1}{x_i-x_{h}} \prod_{h_2=h_2(k_i k_2 \neq j)} \frac{1}{t_j-t_{h}} \tag{23} \]

The following theorem has been proved in reference by Li in [18].

**Theorem 1.** For \( e(x,t) \) defined in (25) and \( \varphi(x,t) \in C^{d+2}[a,b] \times C^{d+2}[0,T], \) we have

\[ |e(x,t)| \leq C [h^{d+1} + r^{d+1}]. \tag{26} \]

**Corollary 1.** For \( e(x,t) \) defined in (25),

\[ \begin{align*}
|e_x(x,t)| & \leq C [h^{d+1} + r^{d+1}], & \varphi(x,t) & \in C^{d+3}[a,b] \times C^{d+2}[0,T], \\
|e_t(x,t)| & \leq C [h^{d+1} + r^{d}], & \varphi(x,t) & \in C^{d+2}[a,b] \times C^{d+3}[0,T], \\
|e_{tt}(x,t)| & \leq C [h^{d-1} + r^{d+1}], & \varphi(x,t) & \in C^{d+4}[a,b] \times C^{d+2}[0,T], d \geq 1.
\end{align*} \tag{27} \]

This corollary can be obtained similarly as Theorem 1, where we omit it.

Let \( \varphi(x,t) \) be the solution of (1) and \( \varphi(x_m,t_n) \) be the numerical solution; then, we have

\[ D\varphi(x_m,t_n) = f(x,t), \tag{28} \]

and

\[ \lim_{m,n \to \infty} D\varphi(x_m,t_n) = f(x,t). \tag{29} \]

According to the above lemma, the following theorem can be proved.

**Theorem 2.** Let \( \varphi(x_m,t_n); D\varphi(x_m,t_n) = f(x,t) \) and \( f(x) \in C[a,b]; \) we have

\[ |\varphi(x,t) - \varphi(x_m,t_n)| \leq C [h^{d+1} + r^{d}], \tag{30} \]

**Proof.** As
Table 1: Convergence rate of equidistant nodes with different $d_1 = 7$ and $t = 2$.

| $n$    | $d_1 = 2$       | $d_1 = 3$       | $d_1 = 4$       | $d_1 = 5$       |
|--------|-----------------|-----------------|-----------------|-----------------|
| $8 \times 8$ | $6.1237 \times 10^1$ | $8.7824 \times 10^1$ | $7.4433 \times 10^1$ | $1.1222 \times 10^2$ |
| $16 \times 16$ | $1.7534 \times 10^1$ | $1.8042$ | $1.0471 \times 10^1$ | $3.0682$ |
| $32 \times 32$ | $3.3624 \times 10^2$ | $2.3828$ | $6.6239 \times 10^3$ | $3.9826$ |
| $64 \times 64$ | $6.0006 \times 10^3$ | $2.4863$ | $4.5724 \times 10^4$ | $3.8567$ |

Table 2: Convergence rate of equidistant nodes with different $d_1 = 7$ and $t = 2$.

| $n$    | $d_1 = 2$       | $d_1 = 3$       | $d_1 = 4$       | $d_1 = 5$       |
|--------|-----------------|-----------------|-----------------|-----------------|
| $8 \times 8$ | $1.677$ | $1.6716$ | $1.6795$ | $1.6782$ |
| $16 \times 16$ | $1.5313 \times 02$ | $6.7751$ | $1.6007 \times 02$ | $6.7064$ |
| $32 \times 32$ | $1.4665 \times 03$ | $3.3843$ | $7.1109 \times 05$ | $7.8144$ |
| $64 \times 64$ | $1.8040 \times 04$ | $3.0231$ | $2.9783 \times 06$ | $4.5775$ |

Table 3: Convergence rate of quasi-equidistant nodes with different $d_1 = 7$ and $t = 2$.

| $n$    | $d_1 = 2$       | $d_1 = 3$       | $d_1 = 4$       | $d_1 = 5$       |
|--------|-----------------|-----------------|-----------------|-----------------|
| $8 \times 8$ | $5.1334 \times 01$ | $3.7631 \times 01$ | $1.1156 \times 01$ | $1.2259 \times 01$ |
| $16 \times 16$ | $2.8133 \times 02$ | $4.1896$ | $1.1572 \times 02$ | $5.0232$ |
| $32 \times 32$ | $2.8913 \times 03$ | $3.2825$ | $5.4800 \times 04$ | $4.4003$ |
| $64 \times 64$ | $3.2935 \times 04$ | $3.1340$ | $3.0820 \times 05$ | $4.1523$ |

Table 4: Convergence rate of quasi-equidistant nodes with different $d_1 = 7$ and $t = 2$.

| $n$    | $d_1 = 2$       | $d_1 = 3$       | $d_1 = 4$       | $d_1 = 5$       |
|--------|-----------------|-----------------|-----------------|-----------------|
| $8 \times 8$ | $2.8707 \times 01$ | $2.8566 \times 01$ | $2.8297 \times 01$ | $2.8323 \times 01$ |
| $16 \times 16$ | $1.0263 \times 02$ | $4.8059$ | $5.7980 \times 04$ | $8.9445$ |
| $32 \times 32$ | $6.1791 \times 04$ | $4.0539$ | $2.9283 \times 06$ | $7.6293$ |
| $64 \times 64$ | $7.9511 \times 04$ | $2.9582$ | $1.3835 \times 06$ | $1.0817$ |

Figure 1: Error estimate of equidistant nodes with $t = 2$, $m = n = 19$, and $d_1 = d_2 = 8$.

\[
D\varphi(x, t) - D\varphi(x_m, t_n) = i\varphi_t(x, t) - \varphi(x, t) + i\varphi_{xx}(x, t) = \left[i\varphi_t(x_m, t_n) - \varphi(x_m, t_n) + i\varphi_{xx}(x_m, t_n)\right]
\]

\[
= i\left[\varphi_t(x, t) - \varphi(x, t)\right] + \left[-\varphi(x, t) + \varphi(x_m, t_n)\right] + i\left[\varphi_{xx}(x, t) - \varphi_{xx}(x_m, t_n)\right]
\]

\[
= iR_1(x, t) + R_2(x, t) + iR_3(x, t),
\]

(31)
Figure 2: Error estimate of quasi-equidistant nodes with $t = 2$, $m = n = 19$, and $d_1 = d_2 = 8$.

Table 5: Convergence rate of equidistant nodes with different $d_1 = 7$ and $t = 1$.

| $n$ | $d_2 = 2$ | $d_2 = 3$ | $d_2 = 4$ | $d_2 = 5$ |
|-----|----------|----------|----------|----------|
| 8 × 8 | 1.7995e-03 | 4.6557e-04 | 1.5050e-04 | 1.4417e-04 |
| 16 × 16 | 5.5795e-04 | 1.6894e-05 | 5.3235e-06 | 3.7235e-06 |
| 32 × 32 | 1.1570e-04 | 2.2698e-05 | 5.9129e-06 | 4.5355e-06 |
| 64 × 64 | 2.1482e-05 | 2.4291e-05 | 7.0393e-06 | 5.6332e-06 |

Table 6: Convergence rate of equidistant nodes with different $d_2 = 7$ and $t = 1$.

| $n$ | $d_1 = 2$ | $d_1 = 3$ | $d_1 = 4$ | $d_1 = 5$ |
|-----|----------|----------|----------|----------|
| 8 × 8 | 1.6168e-03 | 5.1505e-04 | 1.7042e-04 | 9.0483e-05 |
| 16 × 16 | 1.9952e-04 | 3.0185e-05 | 4.5888e-06 | 3.4828e-06 |
| 32 × 32 | 2.5369e-05 | 2.9754e-06 | 4.1516e-07 | 4.1516e-07 |
| 64 × 64 | 3.4030e-06 | 2.8982e-06 | 3.9842e-07 | 5.0649e-07 |

Table 7: Convergence rate of quasi-equidistant nodes with different $d_1 = 7$ and $t = 1$.

| $n$ | $d_2 = 2$ | $d_2 = 3$ | $d_2 = 4$ | $d_2 = 5$ |
|-----|----------|----------|----------|----------|
| 8 × 8 | 2.1572e-03 | 2.1324e-04 | 2.9588e-05 | 1.1861e-05 |
| 16 × 16 | 1.7804e-04 | 3.5989e-05 | 5.0230e-06 | 7.5909e-07 |
| 32 × 32 | 1.2864e-05 | 3.7907e-06 | 4.1551e-07 | 4.2314e-07 |
| 64 × 64 | 1.3676e-06 | 3.2336e-06 | 3.9842e-07 | 8.0913e-08 |

Table 8: Convergence rate of quasi-equidistant nodes with different $d_2 = 7$ and $t = 1$.

| $n$ | $d_1 = 2$ | $d_1 = 3$ | $d_1 = 4$ | $d_1 = 5$ |
|-----|----------|----------|----------|----------|
| 8 × 8 | 2.1937e-03 | 5.6367e-04 | 7.8737e-05 | 6.3534e-06 |
| 16 × 16 | 1.6769e-04 | 3.7094e-05 | 5.9101e-06 | 8.7629e-07 |
| 32 × 32 | 1.4478e-05 | 3.5339e-06 | 4.4821e-07 | 5.5198e-08 |
| 64 × 64 | 7.0252e-06 | 1.0376e-06 | 6.1937e-07 | 1.0710e-06 |
we have
\[
\begin{align*}
R_1(x, t) &= \varphi_1(x, t) - \varphi_1(x_m, t_n), \\
R_2(x, t) &= \varphi_1(x, t) - \varphi(x_m, t_n), \\
R_3(x, t) &= \varphi_{xx}(x, t) - \varphi_{xx}(x_m, t_n).
\end{align*}
\]
(32)

As, for \(R_3(x, t)\), we have
\[
\begin{align*}
R_3(x, t) &= \varphi_{xx}(x, t) - \varphi_{xx}(x_m, t_n) \\
&= \varphi_{xx}(x, t) - \varphi_{xx}(x_m, t_n) + \varphi_{xx}(x, t) - \varphi_{xx}(x_m, t_n) \\
&= \sum_{i=0}^{m-d} (-1)^i \varphi_{xx}[x_{i}, x_{i+1}, \ldots, x_{i+d}, x, t] \\
&+ \sum_{j=0}^{n-d} (-1)^j \varphi_{xx}[t_{j}, t_{j+1}, \ldots, t_{j+d}, x, t] \\
&= e_{xx}(x, t_n) + e_{xx}(x_m, t_n).
\end{align*}
\]
(33)

By the corollary, we obtain
\[
|R_3(x, t)| \leq |e_{xx}(x, t_n) + e_{xx}(x_m, t_n)| \leq C\left(h^{d+1} + r^{d+1}\right).
\]
(34)

Similarly, for \(R_2(x, t)\) and \(R_1(x, t)\), we have
\[
\begin{align*}
R_1(x, t) &= \varphi_1(x, t) - \varphi_1(x_m, t_n) = e_1(x, t_n) - e_1(x_m, t_n), \\
R_2(x, t) &= \varphi_1(x, t) - \varphi(x_m, t_n) = e_1(x, t_n) - e_1(x_m, t_n), \\
|R_1(x, t)| &\leq |e_1(x, t_n) + e_1(x_m, t_n)| \leq C\left(t^{d+1} + r^{d+1}\right),
\end{align*}
\]
(35)

and
\[
|R_2(x, t)| = |\beta\varphi_1(x, t) - \varphi(x_m, t_n)| \leq C\left(h^{d+1} + r^{d+1}\right).
\]
(36)

Combining the identity equations (31), (34), (36), and (37), the conclusion of theorem is obtained.

4. Numerical Examples

Example 1. The SDE \(a = 0, b = 1, t = 2, \) and
\[
f(x, t) = 0,
\]
(38)

under condition \(g_1(x) = \sqrt{2} \sin(\pi x); \) the analysis solution is
\[
\varphi(x, t) = \sqrt{2}e^{-\pi t/2} \sin(\pi x).
\]
(39)

Tables 1 and 2 show the errors of the LBRCM for equidistant nodes of space variables and time variables.

Tables 3 and 4 show the errors of the LBRCM for quasi-equidistant nodes of space variables and time variables.

Example 2. The SDE \(a = 0, b = 1, t = 1, \) and
\[
f(x, t) = (x^2 - 2)e^{\pi t/4} \cos\left(\frac{\pi x}{2}\right) + 2\pi \sin\left(\frac{\pi x}{2}\right),
\]
(40)

under condition \(g_1(x) = x^2 \sin(\pi x/2); \) the analysis solution is
\[
\varphi(x, t) = e^{-t} \sin x.
\]
(41)

In Figures 1 and 2, the error estimate of equidistant and quasi-equidistant nodes with \(t = 2, m = n = 19, \) and \(d_1 = d_2 = 8\) is presented. It can be seen from Figure 2 that the barycentric rational interpolation collocation method has higher accuracy in both quasi-equidistant and equidistant nodes conditions.

Tables 5 and 6 show the errors of the LBRCM for equidistant nodes of space variables and time variables.

Tables 7 and 8 show the errors of the LBRCM for quasi-equidistant nodes of space variables and time variables.

5. Conclusion

In this paper, the LBRCM have been constructed to solve SDE, while the time variable and space variable are obtained at the same time. Numerical solution confirms the theorem analysis.

Data Availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors’ Contributions

This manuscript was written by Peicheng Zhao and Yongling Cheng. Some checks of grammar were given by Yongling Cheng.

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