Exponentially Fitted Symplectic Runge-Kutta-Nyström methods

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Abstract: In this work we consider symplectic Runge Kutta Nyström (SRKN) methods with three stages. We construct a fourth order SRKN with constant coefficients and a trigonometrically fitted SRKN method. We apply the new methods on the two-dimensional harmonic oscillator, the Stiefel-Bettis problem and on the computation of the eigenvalues of the Schrödinger equation.

Keywords: Runge Kutta Nyström methods, symplectic methods, exponential fitting

1. Introduction

Hamiltonian systems are systems of first order ordinary differential equations that can be expressed as

\[ p' = -\frac{\partial H}{\partial q}(p, q, x), \quad q' = \frac{\partial H}{\partial p}(p, q, x), \]

where \((p, q) \in U\) an open subset of \(\mathbb{R}^2\), \(x \in I\) an open subinterval of \(\mathbb{R}\), the integer \(d\) is the number of degrees of freedom. The Hamiltonian function \(H(p, q, x)\) is a twice continuously differentiable function on \(U \times I\) that represents the total mechanical energy. The \(q\) variables are generalized coordinates and the \(p\) variables are the conjugated generalized momenta. The solution operator of a Hamiltonian system is a symplectic transformation.

A symplectic numerical method preserves the symplectic structure in the phase space when applied to Hamiltonian problems. Therefore symplectic numerical methods have been used for the numerical integration of Hamiltonian problems over the past two decades. In this work we shall consider problems with separable Hamiltonian of the special form

\[ H(p, q, x) = \frac{1}{2}p^T p + V(q, x), \]

then the Hamiltonian system has the form

\[ p' = -\frac{\partial}{\partial q} V(q, x), \quad q' = p. \]  \hspace{1cm} (3)

or

\[ q'' = -\frac{\partial}{\partial q} V(q, x). \]  \hspace{1cm} (4)

The last is a system of second order differential equations and have been treated in the literature by Runge-Kutta-Nyström (RKN) and symplectic RKN (SRKN) methods. The theory of these methods can be found in the book of Sanz-Serna and Calvo [4].

On the other hand the solution of Hamiltonian systems often has an oscillatory or periodic behavior and special methods that take into account these properties of the solution have been considered. Among these methods are frequency dependent methods as exponentially, trigonometrically fitted, phase fitted and amplification fitted methods and methods with constant coefficients as minimum phase lag, minimum amplification error, P-stable methods. Exponentially fitted methods integrate exactly differential systems whose solutions can be expressed as linear combinations of functions of the form \(e^{\lambda x}\), \(e^{-\lambda x}\) or \(\sin(\lambda x)\), \(\cos(-\lambda x)\). A detailed survey of these methods can be found in Ixaru and Vanden Berghe. Simos [5] first constructed an exponentially fitted Runge-Kutta method...
that integrates exactly the test equation \( y'' = -w^2 y \). More recently some authors \([2, 3]\) have proposed several exponentially fitted RKN methods. The idea of combining symplecticity with exponential fitting was first introduced by Simos and Aguiar \([6]\) for RKN methods, they presented a two stages modified second order symplectic RKN, also Vyver \([7]\) constructed a two stages modified second order symplectic RKN method that integrates exactly the exponential function at the internal stage also.

Van de Vyver \([8]\) first constructed a symplectic Runge-Kutta-Nyström method with minimum phase-lag. His method has third algebraic order and sixth phase-lag order.

In this work we present two three stages symplectic RKN methods, one with constant coefficients and fourth algebraic order and symplectic modified RKN method which integrates exactly the test equation \( y'' = -w^2 y \) following the approach introduced by Simos. In section two the basic theory of SRKN methods and exponential fitting is presented, the new methods are developed in section 3. Numerical results and conclusions are presented in section 4.

2. Symplectic RKN methods

We consider systems of second order ODEs of the form

\[
y''(x) = f(x, y(x)), \quad x \in [x_0, X],
\]

with initial conditions

\[
y(x_0) = y_0, \quad y'(x_0) = y'_0.
\]

An explicit RKN method is of the form

\[
y_{n+1} = y_n + h y'_n + h^2 \sum_{i=1}^{s} \beta_i f_i,
\]

\[
y'_{n+1} = y'_n + h \sum_{i=1}^{s} b_i f_i,
\]

where

\[
f_i = f \left( x_n + c_i h, y_n + c_i h y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} f_j \right)
\]

and is associated with the Butcher tableau

\[
\begin{array}{cc}
c_1 & a_{11} \\
c_2 & a_{21} \\
c_3 & a_{31} a_{32} \\
\vdots & \vdots \\
c_s & a_{s1} a_{s2} \cdots a_{s,s-1} \\
\hline
\beta_1 & \beta_2 & \cdots & \beta_{s-1} & \beta_s \\
& b_1 & b_2 & \cdots & b_{s-1} & b_s
\end{array}
\]

Suris showed that a RKN method is symplectic when applied to Hamiltonian problems of the form (2) if the coefficients of the method satisfy

\[
\beta_i = b_i (1 - c_i), \quad 1 \leq i \leq s, \tag{6}
\]

\[
b_i (\beta_j - \alpha_{ij}) = b_j (\beta_i - \alpha_{ji}), \quad 1 \leq i, j \leq s. \tag{7}
\]

A RKN method that satisfies (6) and (7) is called symplectic RKN method (SRKN). In the case of explicit RKN methods the coefficients \( a_{ij} \) are fully determined by the coefficients \( b_i \) and \( c_i \)

\[
a_{ij} = b_j (c_i - c_j). \tag{8}
\]

Condition (6) is a well known simplifying assumption from the standard theory of RKN methods that reduces the number of order conditions. Calvo and Sanz-Serna has shown that condition (7) is also a simplifying assumption. The order conditions up to fourth order method are

\[
\begin{align*}
& \text{first order} \\
& b.e = 1, \\
& \text{second order} \\
& b.c.e = \frac{1}{2}, \\
& \text{third order} \\
& b.c^2.e = \frac{1}{3}, \quad b.a.e = \frac{1}{6}, \\
& \text{fourth order} \\
& b.c^3.e = \frac{1}{4}, \quad b.a.c.e = \frac{1}{24}.
\end{align*}
\]

3. Construction of the new methods

We consider the three stage method

\[
\begin{align*}
& c_1 \quad c_2 \quad c_3 \\
& b_1 (c_2 - c_1) \quad b_2 (c_3 - c_2) \quad b_3 (1 - c_3) \\
& b_1 \quad b_2 \quad b_3
\end{align*}
\]

In order to construct the fourth order method we solve the six conditions and derive the following coefficients

\[
\begin{align*}
& b_1 = \frac{3 - 2 \sqrt{3}}{12}, \quad b_2 = \frac{1}{2}, \quad b_3 = \frac{3 + 2 \sqrt{3}}{12}, \\
& c_1 = \frac{3 + \sqrt{3}}{6}, \quad c_2 = \frac{3 - \sqrt{3}}{6}, \quad c_3 = c_1.
\end{align*}
\]

Here we construct new trigonometrically fitted RKN method following the approach introduced by Simos \([5]\) for Runge-Kutta methods. These methods integrate exactly the test equation

\[
y'' = -w^2 y
\]

For the exponentially fitted case we want the numerical method to integrate exactly the exponential function \( \exp(\pm wx) \) with \( w \) real

\[
\exp(\pm v) = 1 \pm v + (\beta.c.e) v^2 \pm (\beta.A.e) v^3 + \beta.A.e v^4 + (\beta.A.C.e) v^5 + (\beta.A.A.e) v^6,
\]

\[
\exp(\pm v) = 1 \pm (b.e) v + (b.C.e) v^2 \pm i(b.A.e) v^3 + (b.A.C.e) v^4 \pm (b.A.A.e) v^5.
\]
where \( v = w h \). For the trignometrically fitted case we want the numerical method to integrate the exponential function \( \exp(iw x) \) with \( w \) real
\[
\exp(iw) = 1 + iw - (\beta.c)e^w - i(\beta.A.e)e^w + i(\beta.A.e)v^5 - (\beta.A.A.e)v^6,
\]
\[
\exp(iv) = 1 + i(b.c)e - (b.c.e)v^2 - i(b.A.e)v^3 + (b.A.C.e)v^4 + i(b.A.A.e)v^5,
\]
or equivalently
\[
\cos v - 1 = - (\beta.e)v^2 + (\beta.A.e)v^4 - (\beta.A.A.e)v^6,
\]
\[
\sin v = 1 - (\beta.c.e)v^2 + (\beta.A.e)v^4,
\]
where
\[
c_3 = 0.73166990421824007504 - 0.01164255863026712775 e^2
\]
\[
-0.000354772795752808874 e^4 - 0.0000250077938624878223 e^6
\]
\[-5.56881613039109410^{-7} e^8 - 5.801982600974105910^{-8} e^{10}.
\]
\[v = \sin v, \quad c = \cos v, \quad b = \beta, \quad A = \alpha, \quad C = \gamma, \quad k = \text{free parameter}.
\]

4. Numerical Results

We shall compare our new methods Meth1 (constant coefficients) and Meth2 (variable coefficients) with the third algebraic order with 6th phase lag order SRKN method of Vyver [8] and the fourth order five stages SRKN method of Calvo and Sanz-Serna.

4.1. The two-dimensional harmonic oscillator

We consider the two-dimensional harmonic oscillator
\[
p_1' = -w_1 q_1, \quad q_1' = p_1, \quad p_2' = -w_2 q_2, \quad q_2' = p_2
\]
with initial conditions
\[
p_1(0) = 0, \quad q_1(0) = 1, \quad p_2(0) = 1, \quad q_2(0) = 0.
\]
The Hamiltonian of this problem is
\[
H(p_1, p_2, q_1, q_2) = T(p_1, p_2) + V(q_1, q_2),
\]
\[
T(p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2),
\]
and
\[
V(q_1, q_2) = \frac{1}{2}(w_1 q_1^2 + w_2 q_2^2).
\]
The exact solution is
\[
q_1(x) = \cos w_1 x, \quad q_2(x) = \sin w_2 x,
\]
we choose \( w_1 = w_2 = 1 \). For this choice we use \( v = h \).
In Table 1 we present the norm of the error in the solution (first line) and the error in the Hamiltonian (second line) for the two-dimensional harmonic oscillator with integration interval [0, 1000] and several stepsizes.

<table>
<thead>
<tr>
<th>h</th>
<th>Meth1</th>
<th>Meth2</th>
<th>Vyver3</th>
<th>CSS4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.10 10^{-8}</td>
<td>4.39 10^{-6}</td>
<td>3.14 10^{-2}</td>
<td>7.52 10^{-2}</td>
</tr>
<tr>
<td>1/2</td>
<td>7.11 10^{-5}</td>
<td>6.66 10^{-15}</td>
<td>3.01 10^{-5}</td>
<td>3.50 10^{-7}</td>
</tr>
<tr>
<td>1/4</td>
<td>2.32 10^{-4}</td>
<td>9.52 10^{-10}</td>
<td>5.36 10^{-4}</td>
<td>4.61 10^{-9}</td>
</tr>
<tr>
<td>1/8</td>
<td>2.26 10^{-7}</td>
<td>1.65 10^{-15}</td>
<td>9.63 10^{-8}</td>
<td>9.87 10^{-10}</td>
</tr>
<tr>
<td>1/16</td>
<td>4.12 10^{-3}</td>
<td>2.39 10^{-13}</td>
<td>1.60 10^{-9}</td>
<td>2.89 10^{-12}</td>
</tr>
</tbody>
</table>

Table 1: The norm of the error in the solution and the error in the Hamiltonian for the two-dimensional harmonic oscillator.
4.2. An orbit problem studied by Stiefel and Bettis

We consider the following almost periodic orbit problem studied by Stiefel and Bettis

\[
\begin{align*}
p_1' &= -q_1 + 0.001 \cos(x), \quad q_1' = p_1, \\
p_2' &= -q_2 + 0.001 \sin(x), \quad q_2' = p_2
\end{align*}
\]

with initial conditions

\[
p_1(0) = 0, \quad q_1(0) = 1, \quad p_2(0) = 0.9995, \quad q_2(0) = 0.
\]

The analytical solution is given by

\[
q(x) = \cos(x) + 0.0005x \sin(x), \\
p(x) = \sin(x) - 0.0005x \cos(x).
\]

In Table 2 we present the norm of the error in the solution for this problem with integration interval \([0, 1000]\) and several step sizes.

<table>
<thead>
<tr>
<th>(h)</th>
<th>(\text{Meth1})</th>
<th>(\text{Meth2})</th>
<th>(\text{Vyver3})</th>
<th>(\text{CSS})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2</td>
<td>2.38 \times 10^{-3}</td>
<td>3.68 \times 10^{-5}</td>
<td>4.66 \times 10^{-5}</td>
<td>4.78 \times 10^{-4}</td>
</tr>
<tr>
<td>1/4</td>
<td>1.42 \times 10^{-3}</td>
<td>2.22 \times 10^{-6}</td>
<td>1.33 \times 10^{-6}</td>
<td>2.98 \times 10^{-4}</td>
</tr>
<tr>
<td>1/8</td>
<td>7.85 \times 10^{-5}</td>
<td>1.38 \times 10^{-7}</td>
<td>1.74 \times 10^{-6}</td>
<td>1.86 \times 10^{-5}</td>
</tr>
<tr>
<td>1/16</td>
<td>5.48 \times 10^{-6}</td>
<td>8.58 \times 10^{-9}</td>
<td>2.19 \times 10^{-7}</td>
<td>1.16 \times 10^{-6}</td>
</tr>
</tbody>
</table>

Table 2: The norm of the error in the solution for the Stiefel-Bettis problem.

4.3. Computation of the eigenvalues of the Schrödinger equation

We shall use our new methods for the purpose of the eigenvalues of the one-dimensional time-independent Schrödinger equation. The Schrödinger equation may be written in the form

\[
-\frac{1}{2} \psi'' + V(x) \psi = E \psi
\]

where \(E\) is the energy eigenvalue, \(V(x)\) the potential, and \(\psi(x)\) the wave function.

4.3.1. The harmonic oscillator

We consider the harmonic oscillator potential

\[
V(x) = \frac{1}{2} k x^2
\]

with boundary conditions \(\psi(-R) = \psi(R) = 0\).

We consider \(k = 1\).

The exact eigenvalues are given by

\[
E_n = n + \frac{1}{2}, \quad n = 0, 1, 2, \ldots
\]

4.3.2. The doubly anharmonic oscillator

The potential of the doubly anharmonic oscillator is

\[
V(x) = \frac{1}{2} x^2 + \lambda_1 x^4 + \lambda_2 x^6
\]

we take \(\lambda_1 = \lambda_2 = 1/2\) The integration interval is \([-R, R]\). In Table 4 we give the computed eigenvalues up to \(E_{20}\) with step \(h = 1/40\) and \(R = 3\).

<table>
<thead>
<tr>
<th>(E)</th>
<th>(\text{Meth1})</th>
<th>(\text{Meth2})</th>
<th>(\text{Vyver3})</th>
<th>(\text{CSS})</th>
</tr>
</thead>
<tbody>
<tr>
<td>54.222484</td>
<td>117</td>
<td>17</td>
<td>3</td>
<td>20</td>
</tr>
<tr>
<td>67.29805</td>
<td>220</td>
<td>25</td>
<td>5</td>
<td>40</td>
</tr>
<tr>
<td>81.262879</td>
<td>384</td>
<td>35</td>
<td>9</td>
<td>71</td>
</tr>
<tr>
<td>96.061534</td>
<td>630</td>
<td>49</td>
<td>13</td>
<td>120</td>
</tr>
<tr>
<td>111.64783</td>
<td>987</td>
<td>64</td>
<td>19</td>
<td>190</td>
</tr>
<tr>
<td>127.982510</td>
<td>1486</td>
<td>81</td>
<td>28</td>
<td>288</td>
</tr>
<tr>
<td>145.031661</td>
<td>2162</td>
<td>102</td>
<td>32</td>
<td>372</td>
</tr>
<tr>
<td>162.765612</td>
<td>3067</td>
<td>123</td>
<td>60</td>
<td>613</td>
</tr>
<tr>
<td>181.158105</td>
<td>–</td>
<td>137</td>
<td>85</td>
<td>829</td>
</tr>
<tr>
<td>200.185694</td>
<td>–</td>
<td>147</td>
<td>121</td>
<td>1123</td>
</tr>
</tbody>
</table>

Table 4: Absolute Error (\(\times 10^{-6}\)) of the eigenvalues of the doubly anharmonic oscillator (\(h = 1/40\)).

We see that the performance of the trigonometrically fitted integrator is superior in comparison to the other methods tested. Furthermore, the computational cost is the same for the three methods with three stages only the 4th order method of Calvo and Sanz-Serma is more expensive.

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References


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