A Sixth-Order A-Stable Explicit One-Step Method for Stiff Systems

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Abstract—This paper presents a sixth-order, explicit, one-step method which is proved to be A-stable. The numerical experiments demonstrate that the new method is suitable for stiff systems.

Keywords—Stiff initial value problems, Numerical analysis, Numerical stability, Numerical solution of ordinary differential equations.

1. INTRODUCTION
The direct Taylor series method, namely, the solution of an initial value problem in ordinary differential equations expanded as a Taylor series, has been considered as both a classical and numerical method (see [1-7], etc.).

The principle of the Taylor series method is totally different from that of other methods in the solution of ODEs. The method, which uses an infinite Taylor series, is A-stable. But, in practice, the series is truncated to M terms, for example, $M = 4, 6, 20, 30, 40$, and beyond. The corresponding real stability intervals are $(-2.78,0)$, $(-3.55,0)$, $(-8.8,0)$, $(-12.6,0)$, and $(-16.3,0)$ for $M = 4, 6, 20, 30, 40$, respectively. None of these is A-stable even though $M$ is very large. On the other hand, when $M$ is large, calculating the derivative may become relatively prohibitive for complicated problems. For this purpose, this paper develops a deformation Taylor series method of sixth-order which is A-stable.

2. FORMATION OF A-STABLE DEFORMATION TAYLOR SERIES METHOD OF SIXTH-ORDER
The problems associated with a stiff system is twofold: stability and accuracy. Based on the characteristics of the solution of a stiff system, the theoretical solution of a stiff system can be represented locally in the interval $[t_n, t_{n+1}]$ by the composition of a polynomial and exponential function of the form

$$PE(t) = a_0 + t \cdot (a_1 + t \cdot (a_2 + t \cdot (a_3 + a_4 \cdot t))) + b_1 \cdot \exp(b_2 \cdot t),$$

where $a_i, i = 0, 1, 2, 3, 4$ and $b_i, i = 1, 2$ are undetermined coefficients.

Now let $y_n$ be an approximation of the theoretical solution at $t_n$ and $f_n = f(t_n, y_n), f^{(i)} = f^{(i)}(t_n, y_n)$, where $f(t, y(t))$ has desired total derivatives, $f^{(i)}(t, y)$ is the $i^{th}$ order derivative of $f$.
Let $f(t, y(t))$, $t_n = nh$ and $h$ be the stepsize. For the initial value problem
\[
y'(t) = f(t, y(t)), \quad t \in [0, T], \quad y(0) = y_0,
\]
integrating both sides of equation (1), we have
\[
y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(t, y(t)) \, dt.
\]
From the pre-designed conditions
\[
y_n = P E(t_n), \quad f_n^{(i)} = P E^{(i)}(t_n), \quad i = 0, 1, 2, 3, 4, 5,
\]
we can deduce a system of algebraic equations of unknown quantities $a_i$ $(i = 0, 1, 2, 3, 4)$ and $b_i (i = 1, 2)$.

\begin{align*}
a_0 + a_1 * t_n + a_2 * t_n * 2 + a_3 * t_n * 3 + a_4 * t_n * 4 + b_1 * \exp(b_2 * t_n) &= y_n, \\
a_1 + 2 * a_2 * t_n + 3 * a_3 * t_n * 2 + 4 * a_4 * t_n * 3 + b_1 * b_2 * \exp(b_2 * t_n) &= f_n, \\
2 * a_2 + 6 * a_3 * t_n + 12 * a_4 * t_n * 2 + b_1 * b_2 * 2 * \exp(b_2 * t_n) &= f_n', \\
6 * a_3 + 24 * a_4 * t_n + b_1 * b_2 * 3 * \exp(b_2 * t_n) &= f_n'', \\
24 * a_4 + b_1 * b_2 * 4 * \exp(b_2 * t_n) &= f_n^3, \\
b_1 * b_2 * 5 * \exp(b_2 * t_n) &= f_n^4, \\
b_1 * b_2 * 6 * \exp(b_2 * t_n) &= f_n^5.
\end{align*}

It is easy to see that, by substitution, we can eliminate the coefficients $a_i$ $(i = 0, 1, 2, 3, 4)$ and $b_i (i = 1, 2)$ provided $f_n^4, f_n^5 \neq 0$. Thus, we can obtain
\[
PE(t) = \left\{ y_n + (t - t_n) * (f_n + (t - t_n)) * \frac{f_n'}{2} + (t - t_n) * \left( \frac{f_n''}{6} + (t - t_n) \right) * \left( \frac{f_n'''}{24} + (t - t_n) \right) \right\} + \frac{f_n^4}{120} \right)
\]

\begin{align*}
+ f_n^5 &\left\{ \exp(z_n * (t - t_n)) - 1 - z_n * (t - t_n) - (z_n * (t - t_n)) * 2 * \frac{1}{2} \\
- (z_n * (t - t_n)) * 3 * \frac{1}{6} - (z_n * (t - t_n)) * 4 * \frac{1}{24} - (z_n * (t - t_n)) * 5 * \frac{1}{120} \right\} / (z_n * 5),
\end{align*}

where $z_n = f_n^5 / f_n^4$. Letting $t = t_{n+1}$, we arrive at
\[
y_{n+1} = y_n + h * \left( f_n + h * \left( \frac{f_n'}{2} + h * \left( \frac{f_n''}{6} + h * \left( \frac{f_n'''}{24} + h * \frac{f_n^4}{120} \right) \right) \right) \right) \\
- f_n^4 * \left( \exp(z_n * h) - 1 - h * z_n * \left( 1 + h * z_n \right) \left( \frac{1}{2} + h * z_n \right) \right) \\
* \left( \frac{1}{6} + h * z_n * \left( \frac{1}{24} + h * \frac{z_n}{120} \right) \right) \right) / (z_n * 5).
\]

Formula (5) can be regarded as a deformation of a sixth-order Taylor series. In fact, a sixth-order Taylor series can be rewritten in the following form:
\[
y_{n+1} = v_n + w_n,
\]
where

\[ v_n = y_n + h \left( f_n + h \left( \frac{f_n}{2} + h \left( \frac{f_n'}{6} + h \left( \frac{f_n''}{24} \right) \right) \right) \right) \]

\[ w_n = h \cdot 5 \cdot \left( \frac{f_n(4)}{120} + h \cdot \frac{f_n(5)}{720} \right). \]

Supposing \( f_n(4) \cdot f_n(5) \neq 0 \) and letting

\[ w_n = f_n(4) \left( \exp(z_n \cdot h) - 1 - h \cdot z_n \left( \frac{1}{2} + h \cdot z_n \left( \frac{1}{6} + h \cdot z_n \right) \right) \right) \]

\[ \cdot \left( \frac{1}{24} + h \cdot z_n \right) / (z_n) \cdot 5, \]

then we have

\[ w_n = h \cdot 5 \cdot \left( \frac{f_n(4)}{120} + h \cdot \frac{f_n(5)}{720} \right) + O(h^7). \]

Thus, it is easy to see that the relationship

\[ w_n = w_n + O(h^7) \]

holds. Therefore formula (5) can be regarded as a deformation of a sixth-order Taylor series from the point of view of having the same order.

### 3. LOCAL TRUNCATION ERROR AND STABILITY OF METHOD (5)

Assume that the solution of the initial value problem (1) has the desired continuous derivatives. The difference operator associated with method (5) is

\[ E[y(t); h] = y(t + h) - y(t) - h \left( y'(t) + h \left( \frac{y''(t)}{2} + h \left( \frac{y'''(t)}{6} + h \cdot \left( \frac{y^{(4)}(t)}{24} + h \cdot \frac{y^{(5)}(t) \cdot h}{120} \right) \right) \right) \right) - y^{(5)}(t) \cdot \left( \exp(h \cdot z(t)) - 1 - h \cdot z(t) \cdot \left( \frac{1}{2} + h \cdot z(t) \cdot \left( \frac{1}{6} + h \cdot z(t) \cdot \frac{1}{24} + h \cdot z(t) \cdot \frac{1}{120} \right) \right) \right) / (z(t) \cdot 5), \]

where \( z(t) = y^{(5)}(t) / y^{(5)}(t) \) and \( y^{(5)}(t) \cdot y^{(6)}(t) \neq 0. \)

If \( E[y(t); h] = O(h^{p+1}) \), we shall say the method has order \( p \). The local truncation error, \( T_{n+1} \), at \( t_{n+1} \) is defined \( E[y(t_n); h] \). It immediately follows, under the usual localization \( y_n = y(t_n) \), that \( y(t_{n+1}) - y_{n+1} = T_{n+1} \).

**Theorem 1.** Suppose that \( y(t) \) is the theoretical solution of the initial value problem (1) and \( y(t) \) is an arbitrary function in \( c^7 \) with \( y^{(5)}(t) \cdot y^{(6)}(t) \neq 0 \) for all \( t \in [0, T] \). Then method (5) has an order of at least 6.

**Proof.** Expanding \( E[y(t); h] \) about \( t = t_n \), we gain

\[ T_{n+1} = \frac{h^7 \left( y^{(7)}(t_n) \cdot z(t_n) \right)}{5040} + O(h^8), \]

indicating that method (5) has an order of at least 6 in general, provided

\[ y^{(5)}(t) \cdot y^{(6)}(t) \neq 0, \quad t \in [0, T]. \]
THEOREM 2. Method (5) is exactly exponentially fitted to order \( r = \infty \) at any point \( \mu = \lambda h \).

PROOF. Applying method (5) to the test equation

\[
y'(t) = \lambda y(t),
\]

\[
y(0) = y_0,
\]

with \( R(\lambda) < 0 \), we find

\[
y_{n+1} = \exp(h\lambda) \cdot y_n,
\]

indicating method (5) is exponentially fitted to order \( r = \infty \) at any point \( \mu = \lambda h \), according to the definition of exponential fitting [8,9].

THEOREM 3. Method (5) gives an exact solution to the test equation (7).

PROOF. For any fixed point \( t = t_n = nh \in [0, T] \), it follows immediately from (8) that

\[
y_n = y_0 \cdot \exp(\lambda t_n).
\]

Thus, for any \( t = t_n \in [0, T] \), we have

\[
y_n = y(t).
\]

This means that method (5) gives an exact solution to the test equation (7).


PROOF. When method (5) is applied to the test equation (7), we get

\[
y_n = \exp(\lambda nh) \cdot y_0.
\]

Since \( \exp(\lambda nh) \to 0 \) as \( n \to \infty \) for all \( \mu = \lambda h \) with \( \Re(\lambda) < 0 \), we have \( y_n \to 0 \) as \( n \to \infty \). Consequently, method (5) is A-stable. It is easy to see from (8) that method (5) is also L-stable. In fact, we have \( Q(h\lambda) = \exp(h\lambda) \) and \( |Q(h\lambda)| \to 0 \) as \( \Re(h\lambda) \to -\infty \).

As stated above, we arrived at an explicit, sixth-order, L-stable one-step method (5).

It is obvious that method (5) is component-applicable to the systems of ODEs.

4. NUMERICAL COMPUTATION

Let us consider some numerical examples. For every example, we arrange the value \( T \) of independent variable, the stepsizes \( h \), the computation step numbers \( N \), the numerical solution, the theoretical solution, and the absolute error \( RN \) of each solution at \( T \). For the numerical results, see Tables 1-5.

EXAMPLE 1. \( y' = -BY + UW \), \( Y(0) = [-1, -1, -1, -1]^T \), where

\[
U = 0.5 \begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix},
\]

\[
B = U \text{diag}(d_1, d_2, d_3, d_4)U, \]

\[
W = (z_1 \ast z_2 \ast z_3 \ast z_4)^T \]

\[
Z = (z_1, z_2, z_3, z_4)^T = UY, \]

\[
D = (d_1, d_2, d_3, d_4)^T = (1000, 800, -10, 0.001)^T.
\]

The theoretical solution of Example 1 is

\[
Y = UZ,
\]
where $Z = (z_1, z_2, z_3, z_4)^T$, $z_i = z_i(t) = d_i/(1 + d_i) \cdot \exp(d_i \cdot t)$, $i = 1, 2, 3, 4$. For the numerical results, see Table 1.

EXAMPLE 2.

$$
\begin{align*}
    y_1' &= -1002 \cdot y_1 + 1000 \cdot y_2 \cdot y_2, \quad y_1(0) = 1, \\
    y_2' &= y_1 - y_2 \cdot (1 + y_2), \quad y_2(0) = 1.
\end{align*}
$$

The theoretical solution of Example 2 is

$$
\begin{align*}
    y_1 &= \exp(-2t), \\
    y_2 &= \exp(-t).
\end{align*}
$$

For the numerical results, see Table 2.

EXAMPLE 3.

$$
\begin{align*}
    y_1' &= -20 \cdot y_1 - 0.25 \cdot y_2 - 19.75 \cdot y_3, \quad y_1(0) = 1, \\
    y_2' &= 20 \cdot y_1 - 20.25 \cdot y_2 + 0.25 \cdot y_3, \quad y_2(0) = 0, \\
    y_3' &= 20 \cdot y_1 - 19.75 \cdot y_2 - 0.25 \cdot y_3, \quad y_3(0) = -1.
\end{align*}
$$

The theoretical solution of Example 3 is

$$
\begin{align*}
    y_1 &= \frac{\left[\exp(-0.5t) + \exp(-20t) \cdot (\cos(20t) + \sin(20t))\right]}{2}, \\
    y_2 &= \frac{\left[\exp(-0.5t) - \exp(-20t) \cdot (\cos(20t) - \sin(20t))\right]}{2}, \\
    y_3 &= -\frac{\left[\exp(-0.5t) + \exp(-20t) \cdot (\cos(20t) - \sin(20t))\right]}{2}.
\end{align*}
$$

For the numerical results, see Table 3.
EXAMPLE 4.

\[ y_1' = -0.1 \cdot y_1 - 49.9 \cdot y_2, \quad y_1(0) = 2, \]
\[ y_2' = -50 \cdot y_2, \quad y_2(0) = 1, \]
\[ y_3' = 70 \cdot y_2 - 120 \cdot y_3, \quad y_3(0) = 2. \]

The theoretical solution of Example 4 is

\[ y_1 = \exp(-0.1t) + \exp(-50t), \]
\[ y_2 = \exp(-50t), \]
\[ y_3 = \exp(-50t) + \exp(-120t). \]

For the numerical results, see Table 4.

<table>
<thead>
<tr>
<th>( T )</th>
<th>( h )</th>
<th>( N )</th>
<th>( Y )</th>
<th>Numerical</th>
<th>Theoretical</th>
<th>( RN )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.025</td>
<td>400</td>
<td>( y_1 )</td>
<td>0.36789441171</td>
<td>0.36789441171</td>
<td>2.44E - 15</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( y_2 )</td>
<td>0.712457640674E - 217</td>
<td>0.712457650681E - 217</td>
<td>2.63E - 229</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( y_3 )</td>
<td>0.712457640674E - 217</td>
<td>0.712457640674E - 217</td>
<td>2.63E - 229</td>
</tr>
</tbody>
</table>

EXAMPLE 5. Consider the following Van der Pol equation:

\[ x'' - 50 \cdot (1 - x \cdot x) \cdot x' + x = 0, \quad x(0) = 2.002945, \quad x'(0) = 0. \]

For the numerical results, see Table 5.

<table>
<thead>
<tr>
<th>( T/2 )</th>
<th>( h )</th>
<th>( N )</th>
<th>( Y )</th>
<th>Numerical</th>
<th>Theoretical</th>
<th>( RN )</th>
</tr>
</thead>
<tbody>
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<td>41.253</td>
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<td>41253</td>
<td>( x )</td>
<td>-2.0029450032</td>
<td>-2.002945</td>
<td>3.2E - 9</td>
</tr>
</tbody>
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REFERENCES