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Two-stage Explicit Runge-Kutta Type Methods Using Derivatives

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Two-stage explicit Runge-Kutta type methods using derivatives for the system $y'(t) = f(y(t))$, $y(t_0) = y_0$ are considered. Derivatives in the first stage have the standard form, but in the second stage, they have the form included in the limiting formula. The kth-order Taylor series method uses derivatives f', $f'', \ldots, f^{(k-1)}$. Though the values of derivatives can be easily obtained by using automatic differentiation, the cost increases proportional to square of the order of differentiation. Two-stage methods considered here use the derivatives up to $f^{(k-3)}$ in the first stage and f, f' in the second stage. They can achieve kth-order accuracy and construct embedded formula for the error estimation.

Key words: Runge-Kutta method, higher order method, automatic differentiation, embedded formula

1. Introduction

We will consider two-stage explicit Runge-Kutta type methods using derivatives for the initial value problem

$$\frac{d}{dt}y(t) = f(y(t)), \quad y(t_0) = y_0 \tag{1}$$

where y and f are vectors and f is assumed to be sufficiently smooth.

Previously, one of the authors reported a Runge-Kutta type method using second derivatives, which was a two-stage method and achieved fourth-order accuracy with embedded third-order formula [10]. Also, the authors proposed a two-stage Runge-Kutta type method, which used the third derivatives in the first stage and achieved fifth-order accuracy with embedded fourth-order formulas [14].

Here, we present a generalized two-stage method using derivatives up to $f^{(k-3)}$ in the first stage and f, f' in the second stage. The derivative f' in the second stage is in the form appeared in the limiting formula [8, 9, 12]. We show that the method can achieve kth-order accuracy with embedded $(k-1)$th-order formulas.

The kth-order Taylor series method uses derivatives up to $f^{(k-1)}$. Though the values of derivatives can be easily obtained by using automatic differentiation [5, 11, 13], the cost increases proportional to square of the order of differentiation. From this viewpoint, the proposed method is more efficient than the kth-order

Taylor series method.

In the following section we introduce general formula which illustrates the method, and solve the order conditions. Then we show that there remains one free parameter. We propose a value of the free parameter for minimizing the leading truncation errors.

Section three presents numerical examples and conclusions.

2. Two-stage Method Using Derivatives of Higher Order

In this section we present a general formula for the proposed method, and then derive the order conditions. We show that the formula can not be $(k+1)$th-order and the order conditions for kth-order are solved with one free parameter. Next, we propose a $(k-1)$th-order formula which is embedded in the kth-order formula with the free parameter. Then, we investigate the leading truncation error terms of these formulas. This is followed by a discussion of the values of the free parameter for minimizing the truncation errors.

2.1. General form

We will consider the formula

$$
\begin{aligned}
f_1 &= f(y_n) = f(y(t_n)), \\
\dot{f}_1 &= \left(\frac{d}{dt} f(y(t))\right)_{t=t_n} = \left(\frac{d^2 y}{dt^2}\right)_{t=t_n}, \\
\ddot{f}_1 &= \left(\frac{d^2}{dt^2} f(y(t))\right)_{t=t_n} = \left(\frac{d^3 y}{dt^3}\right)_{t=t_n}, \\
&\cdots \\
\overset{\cdot(k-3)}{f_1} &= \left(\frac{d^{k-3}}{dt^{k-3}} f(y(t))\right)_{t=t_n} = \left(\frac{d^{k-2} y}{dt^{k-2}}\right)_{t=t_n}, \\
y_{c_2} &= y_n + hc_2 f_1 + \frac{(hc_2)^2}{2!}\dot{f}_1 + \frac{(hc_2)^3}{3!}\ddot{f}_1 + \cdots + \frac{(hc_2)^{k-2}}{(k-2)!}\overset{\cdot(k-3)}{f_1}, \\
f_2 &= f(y_{c_2}), \\
\tilde{f}_2 &= f_2 + \gamma\left(f_1 + hc_2\dot{f}_1 + \frac{(hc_2)^2}{2!}\ddot{f}_1 + \cdots + \frac{(hc_2)^{k-3}}{(k-3)!}\overset{\cdot(k-3)}{f_1}\right), \\
\dot{\tilde{f}}_2 &= \left(\frac{\partial f}{\partial y}\right)_{y=y_{c_2}} \cdot \tilde{f}_2, \\
\hat{y}_{n+1} &= y_n + h(\hat{b}_1 f_1 + \hat{b}_2 f_2) + h^2(\hat{\bar{b}}_1 \dot{f}_1 + \hat{\bar{b}}_2 \dot{\tilde{f}}_2) \\
&\quad + h^3 \hat{\bar{\bar{b}}}_1 \ddot{f}_1 + \cdots + h^{k-2}\, \hat{\overset{(k-3)}{\bar{b}_1}}\, \overset{\cdot(k-3)}{f_1}, \\
y_{n+1} &= y_n + h(b_1 f_1 + b_2 f_2) + h^2(\bar{b}_1 \dot{f}_1 + \bar{b}_2 \dot{\tilde{f}}_2) \\
&\quad + h^3 \bar{\bar{b}}_1 \ddot{f}_1 + \cdots + h^{k-2}\, \overset{(k-3)}{\bar{b}_1}\, \overset{\cdot(k-3)}{f_1},
\end{aligned} \tag{2}
$$

$$E = y_{n+1} - \hat{y}_{n+1}$$

where y and f are vectors, $\hat{y}_{n+1}$ is a lower order formula embedded in y_{n+1}, and, E is an estimation of the truncation error of $\hat{y}_{n+1}$. We refer to the product $\tilde{\dot{f}}_2$ as a second-order pseudo-derivative.

2.2. Equations of order condition and solutions

Using the expansion of true value

$$(3) \qquad y(t_n + hc_2) = y_n + hc_2 f_1 + \frac{(hc_2)^2}{2!}\dot{f}_1 + \frac{(hc_2)^3}{3!}\ddot{f}_1 + \cdots + \frac{(hc_2)^{k-2}}{(k-2)!}\overset{\cdot(k-3)}{f_1} + \frac{(hc_2)^{k-1}}{(k-1)!}\overset{\cdot(k-2)}{f_1} + \frac{(hc_2)^{k}}{k!}\overset{\cdot(k-1)}{f_1} + \cdots,$$

we can write

$$(4) \qquad y_{c_2} = y(t_n + hc_2) - R_{k-1}$$

where

$$(5) \qquad R_{k-1} = \frac{(hc_2)^{k-1}}{(k-1)!}\overset{\cdot(k-2)}{f_1} + \frac{(hc_2)^{k}}{k!}\overset{\cdot(k-1)}{f_1} + \cdots .$$

The expansion of f_2 can be obtained by using (4) as follows:

$$(6) \qquad f_2 = f(y_{c_2}) = f(y(t_n + hc_2) - R_{k-1}) = f(y(t_n + hc_2)) - \left(\frac{\partial f}{\partial y}\right)_{y=y(t_n+hc_2)} \cdot R_{k-1} + \cdots .$$

The first term of the expression (6) becomes, from (3),

$$(7) \qquad f(y(t_n + hc_2)) = f_1 + hc_2\dot{f}_1 + \frac{(hc_2)^2}{2!}\ddot{f}_1 + \cdots + \frac{(hc_2)^{k-2}}{(k-2)!}\overset{\cdot(k-2)}{f_1} + \frac{(hc_2)^{k-1}}{(k-1)!}\overset{\cdot(k-1)}{f_1} + \frac{(hc_2)^{k}}{k!}\overset{\cdot(k)}{f_1} + \cdots .$$

The Jacobian matrix in (6) can be written, using the summation convention, as follows:

$$(8) \qquad \left(\frac{\partial f}{\partial y^j}\right)_{y=y(t_n+hc_2)} = \left(\frac{\partial f}{\partial y^j}\right)_{y=y_n+(hc_2 f_1+\cdots)} = \left(\frac{\partial f}{\partial y^j}\right)_{y=y_n} + \left(\frac{\partial^2 f}{\partial y^j \partial y^l}\right)_{y=y_n} (hc_2 f_1^l + \cdots),$$

where y^j denotes the j-th component of the vector y.

We introduce the following notation of elementary differentials shown in [3],

$$\mathbf{f}_j = \left(\frac{\partial f}{\partial y^j}\right)_{y=y_n},$$
$$\mathbf{f}_{jl} = \left(\frac{\partial^2 f}{\partial y^j \partial y^l}\right)_{y=y_n},$$
$$\cdots .$$

Using this notation, the Jacobian matrix is represented as

$$\left(\frac{\partial f}{\partial y^j}\right)_{y=y(t_n+hc_2)} = \mathbf{f}_j + hc_2 \mathbf{f}_{jl} f_1^l + \cdots . \tag{9}$$

Then, we obtain the expansion of the second term of (6) as

$$\begin{aligned}
&\left(\frac{\partial f}{\partial y}\right)_{y=y(t_n+hc_2)} \cdot R_{k-1} \\
&= (\mathbf{f}_j + hc_2\mathbf{f}_{jl}f_1^l + \cdots)\left(\frac{(hc_2)^{k-1}}{(k-1)!}\overset{\cdot(k-2)}{f_1^j} + \frac{(hc_2)^k}{k!}\overset{\cdot(k-1)}{f_1^j} + \cdots\right) \\
&= \frac{(hc_2)^{k-1}}{(k-1)!}\mathbf{f}_j \overset{\cdot(k-2)}{f_1^j} + \frac{(hc_2)^k}{k!}\left(\mathbf{f}_j \overset{\cdot(k-1)}{f_1^j} + k\,\mathbf{f}_{jl} \overset{\cdot(k-2)}{f_1^j} f_1^l\right) + \cdots .
\end{aligned} \tag{10}$$

Substituting (7) and (10) into (6), we obtain

$$\begin{aligned}
f_2 = {} & f_1 + hc_2\dot{f}_1 + \frac{(hc_2)^2}{2!}\ddot{f}_1 + \cdots + \frac{(hc_2)^{k-2}}{(k-2)!}\overset{\cdot(k-2)}{f_1} \\
&+ \frac{(hc_2)^{k-1}}{(k-1)!}\left(\overset{\cdot(k-1)}{f_1} - \mathbf{f}_j \overset{\cdot(k-2)}{f_1^j}\right) \\
&+ \frac{(hc_2)^k}{k!}\left(\overset{\cdot(k)}{f_1} - \mathbf{f}_j \overset{\cdot(k-1)}{f_1^j} - k\,\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j} f_1^l\right) + \cdots .
\end{aligned} \tag{11}$$

Next, using (11), $\tilde{f}_2$ can be written as

$$\begin{aligned}
\tilde{f}_2 &= f_2 + \gamma\left(f_1 + hc_2\dot{f}_1 + \frac{(hc_2)^2}{2!}\ddot{f}_1 + \cdots + \frac{(hc_2)^{k-3}}{(k-3)!}\overset{\cdot(k-3)}{f_1}\right) \\
&= (1+\gamma)\left(f_1 + hc_2\dot{f}_1 + \frac{(hc_2)^2}{2!}\ddot{f}_1 + \cdots + \frac{(hc_2)^{k-3}}{(k-3)!}\overset{\cdot(k-3)}{f_1}\right) \\
&\quad + \frac{(hc_2)^{k-2}}{(k-2)!}\overset{\cdot(k-2)}{f_1} + \frac{(hc_2)^{k-1}}{(k-1)!}\left(\overset{\cdot(k-1)}{f_1} - \mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\right) + \cdots \\
&= (1+\gamma)\left(f(y(t_n+hc_2)) - \frac{(hc_2)^{k-2}}{(k-2)!}\overset{\cdot(k-2)}{f_1} - \frac{(hc_2)^{k-1}}{(k-1)!}\overset{\cdot(k-1)}{f_1} - \cdots\right) \\
&\quad + \frac{(hc_2)^{k-2}}{(k-2)!}\overset{\cdot(k-2)}{f_1} + \frac{(hc_2)^{k-1}}{(k-1)!}\left(\overset{\cdot(k-1)}{f_1} - \mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\right) + \cdots
\end{aligned} \tag{12}$$

$$= (1+\gamma)f(y(t_n+hc_2)) - \frac{(hc_2)^{k-2}}{(k-2)!}\gamma \overset{\cdot(k-2)}{f_1}$$

$$- \frac{(hc_2)^{k-1}}{(k-1)!}\left(\gamma \overset{\cdot(k-1)}{f_1} + \mathbf{f}_j \overset{\cdot(k-2)}{f_1^j}\right) + \cdots .$$

Using (4) and (5), we obtain the expansion of Jacobian matrix at the point y_{c_2} as

$$\text{(13)} \quad \left(\frac{\partial f}{\partial y^j}\right)_{y=y_{c_2}} = \left(\frac{\partial f}{\partial y^j}\right)_{y=y(t_n+hc_2)-R_{k-1}}$$

$$= \left(\frac{\partial f}{\partial y^j}\right)_{y=y(t_n+hc_2)} - \left(\frac{\partial^2 f}{\partial y^j \partial y^l}\right)_{y=y(t_n+hc_2)} \cdot R^l_{k-1} + \cdots$$

$$= \left(\frac{\partial f}{\partial y^j}\right)_{y=y(t_n+hc_2)} - \frac{(hc_2)^{k-1}}{(k-1)!}\mathbf{f}_{jl} \overset{\cdot(k-2)}{f_1^l} + \cdots .$$

Then, from (12) and (13) we obtain

$$\text{(14)} \quad \tilde{\tilde{f}}_2 = \left(\frac{\partial f}{\partial y}\right)_{y=y_{c_2}} \cdot \tilde{f}_2$$

$$= \left[\left(\frac{\partial f}{\partial y^j}\right)_{y=y(t_n+hc_2)} - \frac{(hc_2)^{k-1}}{(k-1)!}\mathbf{f}_{jl} \overset{\cdot(k-2)}{f_1^l} + \cdots\right]$$

$$\times \left[(1+\gamma)f^j(y(t_n+hc_2)) - \frac{(hc_2)^{k-2}}{(k-2)!}\gamma \overset{\cdot(k-2)}{f_1^j}\right.$$

$$\left. - \frac{(hc_2)^{k-1}}{(k-1)!}\left(\gamma \overset{\cdot(k-1)}{f_1^j} + \mathbf{f}^j_l \overset{\cdot(k-2)}{f_1^l}\right) + \cdots\right]$$

$$= (1+\gamma)\left(\frac{\partial f}{\partial y}\right)_{y=y(t_n+hc_2)} \cdot f(y(t_n+hc_2))$$

$$- \left(\frac{\partial f}{\partial y}\right)_{y=y(t_n+hc_2)} \cdot \left[\frac{(hc_2)^{k-2}}{(k-2)!}\gamma \overset{\cdot(k-2)}{f_1}\right.$$

$$\left. + \frac{(hc_2)^{k-1}}{(k-1)!}\left(\gamma \overset{\cdot(k-1)}{f_1} + \mathbf{f}_l \overset{\cdot(k-2)}{f_1^l}\right) + \cdots\right]$$

$$- \frac{(hc_2)^{k-1}}{(k-1)!}(1+\gamma)\mathbf{f}_{jl} \overset{\cdot(k-2)}{f_1^l} f^j(y(t_n+hc_2)) + \cdots .$$

The first term of the last expression of (14) becomes, from (7),

$$\text{(15)} \quad \left(\frac{\partial f}{\partial y}\right)_{y=y(t_n+hc_2)} \cdot f(y(t_n+hc_2)) = \left(\frac{d^2y}{dt^2}\right)_{t=t_n+hc_2}$$

$$= \left(\frac{d^2y}{dt^2} + hc_2\frac{d^3y}{dt^3} + \frac{(hc_2)^2}{2!}\frac{d^4y}{dt^4} + \cdots\right.$$

$$\left. + \frac{(hc_2)^{k-2}}{(k-2)!}\frac{d^ky}{dt^k} + \frac{(hc_2)^{k-1}}{(k-1)!}\frac{d^{(k+1)}y}{dt^{(k+1)}} + \cdots\right)_{t=t_n}$$

$$= \dot{f}_1 + hc_2\ddot{f}_1 + \frac{(hc_2)^2}{2!}\dddot{f}_1 + \cdots + \frac{(hc_2)^{k-2}}{(k-2)!}\overset{\cdot(k-1)}{f_1} + \frac{(hc_2)^{k-1}}{(k-1)!}\overset{\cdot(k)}{f_1} + \cdots,$$

the second term becomes, from (8),

$$(16)\quad \left(\frac{\partial f}{\partial y}\right)_{y=y(t_n+hc_2)} \cdot \left[\frac{(hc_2)^{k-2}}{(k-2)!}\gamma\overset{\cdot(k-2)}{f_1} + \frac{(hc_2)^{k-1}}{(k-1)!}\left(\gamma\overset{\cdot(k-1)}{f_1} + \mathbf{f}_l\overset{\cdot(k-2)}{f_1^l}\right) + \cdots\right]$$

$$= \left[\mathbf{f}_j + hc_2\mathbf{f}_{jl}f_1^l + \cdots\right]\left[\frac{(hc_2)^{k-2}}{(k-2)!}\gamma\overset{\cdot(k-2)}{f_1^j} + \frac{(hc_2)^{k-1}}{(k-1)!}\left(\gamma\overset{\cdot(k-1)}{f_1^j} + \mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l}\right) + \cdots\right]$$

$$= \frac{(hc_2)^{k-2}}{(k-2)!}\gamma\mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}$$

$$+ \frac{(hc_2)^{k-1}}{(k-1)!}\left(\gamma\mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} + \mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l} + (k-1)\gamma\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}f_1^l\right) + \cdots,$$

and the last term becomes, from (7),

$$(17)\quad \frac{(hc_2)^{k-1}}{(k-1)!}(1+\gamma)\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}\cdot f^l(y(t_n+hc_2))$$

$$= \frac{(hc_2)^{k-1}}{(k-1)!}(1+\gamma)\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}\left(f_1^l + hc_2\dot{f}_1{}^l + \cdots\right)$$

$$= \frac{(hc_2)^{k-1}}{(k-1)!}(1+\gamma)\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}f_1^l + \cdots.$$

Substituting (15), (16) and (17) into (14), we obtain

$$(18)\quad \tilde{\dot{f}}_2 = (1+\gamma)\left(\dot{f}_1 + hc_2\ddot{f}_1 + \frac{(hc_2)^2}{2!}\dddot{f}_1 + \cdots + \frac{(hc_2)^{k-3}}{(k-3)!}\overset{\cdot(k-2)}{f_1}\right.$$

$$\left. + \frac{(hc_2)^{k-2}}{(k-2)!}\overset{\cdot(k-1)}{f_1} + \frac{(hc_2)^{k-1}}{(k-1)!}\overset{\cdot(k)}{f_1} + \cdots\right)$$

$$- \left(\frac{(hc_2)^{k-2}}{(k-2)!}\gamma\mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\right.$$

$$\left. + \frac{(hc_2)^{k-1}}{(k-1)!}\left(\gamma\mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} + \mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l} + (k-1)\gamma\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}f_1^l\right) + \cdots\right)$$

$$- \frac{(hc_2)^{k-1}}{(k-1)!}(1+\gamma)\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}f_1^l + \cdots$$

$$= (1+\gamma)\left(\dot{f}_1 + hc_2\ddot{f}_1 + \frac{(hc_2)^2}{2!}\dddot{f}_1 + \cdots + \frac{(hc_2)^{k-3}}{(k-3)!}\overset{\cdot(k-2)}{f_1}\right)$$

$$+ \frac{(hc_2)^{k-2}}{(k-2)!}\left((1+\gamma)\overset{\cdot(k-1)}{f_1} - \gamma\mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\right)$$

$$+ \frac{(hc_2)^{k-1}}{(k-1)!}\left((1+\gamma)\overset{\cdot(k)}{f_1} - \gamma\mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - \mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l} - (1+k\gamma)\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}f_1^l\right) + \cdots$$

$$
\begin{aligned}
&= (1+\gamma)\left(\dot{f}_1 + hc_2\ddot{f}_1 + \frac{(hc_2)^2}{2!}\dddot{f}_1 + \cdots + \frac{(hc_2)^{k-3}}{(k-3)!}\overset{\cdot(k-2)}{f_1}\right)\\
&\quad + \frac{(hc_2)^{k-2}}{(k-2)!}\left((1+\gamma)\Big(\overset{\cdot(k-1)}{f_1} - \mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\Big) + \mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\right)\\
&\quad + \frac{(hc_2)^{k-1}}{(k-1)!}\left((1+\gamma)\Big(\overset{\cdot(k)}{f_1} - \mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - k\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}f_1^l\Big)\right.\\
&\qquad \left. + \Big(\mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - \mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l} + (k-1)\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}f_1^l\Big)\right) + \cdots.
\end{aligned}
$$

Finally, by using (11) and (18), we obtain the expansion of y_{n+1}:

$$
\begin{aligned}
(19)\quad y_{n+1} &= y_n + h(b_1f_1 + b_2f_2) + h^2(\bar{b}_1\dot{f}_1 + \bar{b}_2\tilde{\dot{f}}_2)\\
&\quad + h^3\,\bar{\bar{b}}_1\,\ddot{f}_1 + \cdots + h^{k-2}\,\overset{(k-3)}{\bar{b}_1}\,\overset{\cdot(k-3)}{f_1}\\
&= y_n + h(b_1+b_2)f_1 + h^2(b_2c_2 + \bar{b}_1 + \bar{b}_2(1+\gamma))\dot{f}_1\\
&\quad + h^3\left(\frac{b_2c_2^2}{2!} + \bar{\bar{b}}_1 + \bar{b}_2(1+\gamma)c_2\right)\ddot{f}_1 + \cdots\\
&\quad + h^{k-2}\left(\frac{b_2c_2^{k-3}}{(k-3)!} + \overset{(k-3)}{\bar{b}_1} + \bar{b}_2(1+\gamma)\frac{c_2^{k-4}}{(k-4)!}\right)\overset{\cdot(k-3)}{f_1}\\
&\quad + h^{k-1}\left(\frac{b_2c_2^{k-2}}{(k-2)!} + \bar{b}_2(1+\gamma)\frac{c_2^{k-3}}{(k-3)!}\right)\overset{\cdot(k-2)}{f_1}\\
&\quad + h^{k}\left[\left(\frac{b_2c_2^{k-1}}{(k-1)!} + \bar{b}_2(1+\gamma)\frac{c_2^{k-2}}{(k-2)!}\right)\Big(\overset{\cdot(k-1)}{f_1} - \mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\Big)\right.\\
&\qquad \left. + \frac{\bar{b}_2c_2^{k-2}}{(k-2)!}\mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\right]\\
&\quad + h^{k+1}\left[\left(\frac{b_2c_2^{k}}{k!} + \bar{b}_2(1+\gamma)\frac{c_2^{k-1}}{(k-1)!}\right)\Big(\overset{\cdot(k)}{f_1} - \mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - k\,\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}f_1^l\Big)\right.\\
&\qquad \left. + \frac{\bar{b}_2c_2^{k-1}}{(k-1)!}\Big(\mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - \mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l} + (k-1)\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}f_1^l\Big)\right] + \cdots.
\end{aligned}
$$

The Taylor expansion of $y(t_n + h)$ is as follows:

$$
\begin{aligned}
(20)\qquad y(t_n+h) &= y_n + hf_1 + \frac{h^2}{2!}\dot{f}_1 + \frac{h^3}{3!}\ddot{f}_1 + \cdots + \frac{h^{k-2}}{(k-2)!}\overset{\cdot(k-3)}{f_1}\\
&\quad + \frac{h^{k-1}}{(k-1)!}\overset{\cdot(k-2)}{f_1} + \frac{h^k}{k!}\overset{\cdot(k-1)}{f_1} + \frac{h^{k+1}}{(k+1)!}\overset{\cdot(k)}{f_1} + \cdots.
\end{aligned}
$$

The coefficients of h^k term and $h^{(k+1)}$ term of (20) are represented as

$$
(21)\qquad \frac{1}{k!}\overset{\cdot(k-1)}{f_1} = \frac{1}{k!}\Big(\overset{\cdot(k-1)}{f_1} - \mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\Big) + \frac{1}{k!}\mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}
$$

$$\text{(22)}\qquad \frac{1}{(k+1)!}\overset{\cdot(k)}{f_1} = \frac{1}{(k+1)!}\Big(\overset{\cdot(k)}{f_1} - \mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - k\,\mathbf{f}_{jl}f_1^l\overset{\cdot(k-2)}{f_1^j}\Big) + \frac{1}{(k+1)!}\mathbf{f}_j\Big(\overset{\cdot(k-1)}{f_1^j} - \mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l}\Big) + \frac{k}{(k+1)!}\mathbf{f}_{jl}f_1^l\overset{\cdot(k-2)}{f_1^j} + \frac{1}{(k+1)!}\mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l}\,.$$

The fourth term $\mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l}$ of the right side expression in (22) does not appear in the expansion of y_{n+1} (19), therefore the formula (2) can not be $(k+1)$th-order.

We obtain the following equations of order condition for kth-order formula:

$$\text{(23)}\qquad \begin{aligned}
hf_1 &: b_1+b_2 &&= 1,\\
h^2\dot{f}_1 &: b_2c_2+\bar{b}_2(1+\gamma)+\bar{b}_1 &&= \frac{1}{2!},\\
h^3\ddot{f}_1 &: b_2\frac{c_2^2}{2!}+\bar{b}_2(1+\gamma)c_2+\bar{\bar{b}}_1 &&= \frac{1}{3!},\\
h^4\dddot{f}_1 &: b_2\frac{c_2^3}{3!}+\bar{b}_2(1+\gamma)\frac{c_2^2}{2!}+\bar{\bar{\bar{b}}}_1 &&= \frac{1}{4!},\\
&\cdots\\
h^{k-2}\overset{\cdot(k-3)}{f_1} &: b_2\frac{c_2^{k-3}}{(k-3)!}+\bar{b}_2(1+\gamma)\frac{c_2^{k-4}}{(k-4)!}+\overset{(k-3)}{\bar{b}_1} &&= \frac{1}{(k-2)!},\\
h^{k-1}\overset{\cdot(k-2)}{f_1} &: b_2\frac{c_2^{k-2}}{(k-2)!}+\bar{b}_2(1+\gamma)\frac{c_2^{k-3}}{(k-3)!} &&= \frac{1}{(k-1)!},\\
h^k\Big(\overset{\cdot(k-1)}{f_1}-\mathbf{f}_j\overset{\cdot(k-2)}{f_1^j}\Big) &: b_2\frac{c_2^{k-1}}{(k-1)!}+\bar{b}_2(1+\gamma)\frac{c_2^{k-2}}{(k-2)!} &&= \frac{1}{k!},\\
h^k\mathbf{f}_j\overset{\cdot(k-2)}{f_1^j} &: \bar{b}_2\frac{c_2^{k-2}}{(k-2)!} &&= \frac{1}{k!}.
\end{aligned}$$

From this system of equations, we obtain a solution with a free parameter c_2 for kth-order formula:

$$\text{(24)}\qquad \bar{b}_2 = \frac{1}{k(k-1)c_2^{k-2}},$$

$$\text{(25)}\qquad b_2 = \frac{kc_2-(k-2)}{kc_2^{k-1}},\qquad \gamma = k-2-kc_2,$$
$$b_1 = 1-b_2,$$

$$\text{(26)}\qquad \overset{(l)}{\bar{b}_1} = \frac{1}{(l+1)!} - b_2\frac{c_2^l}{l!} - \bar{b}_2(1+\gamma)\frac{c_2^{l-1}}{(l-1)!}\quad (l=1,2,\ldots,k-3).$$

2.3. Embedded formula

The embedded $(k-1)$-th order formula $\hat{y}_{n+1}$ is defined in (2). We obtain the parameters for the formula using equations up to $h^{(k-1)}$ term in (23) as follows:

$$\hat{b}_2 = \frac{1}{(k-1)c_2^{k-2}}\left(1 - \frac{\hat{\bar{b}}_2}{\bar{b}_2}\frac{(k-2)(k-1-kc_2)}{kc_2}\right), \tag{27}$$

$$\hat{b}_1 = 1 - \hat{b}_2,$$

$$\overset{\widehat{(l)}}{\bar{b}_1} = \frac{1}{(l+1)!} - \hat{b}_2\frac{c_2^l}{l!} - \hat{\bar{b}}_2(1+\gamma)\frac{c_2^{l-1}}{(l-1)!} \quad (l = 1, 2, \ldots, k-3). \tag{28}$$

2.4. Leading term of the local truncation error

From (19) and (20), the coefficient of leading truncation error term of k-th order formula is as follows:

$$\begin{aligned}
&\left(\frac{b_2c_2^k}{k!} + \bar{b}_2(1+\gamma)\frac{c_2^{k-1}}{(k-1)!}\right)\left(\overset{\cdot(k)}{f_1} - \mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - k\,\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}\,f_1^l\right) \\
&\quad + \frac{\bar{b}_2c_2^{k-1}}{(k-1)!}\left(\mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - \mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l} + (k-1)\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}\,f_1^l\right) - \frac{1}{(k+1)!}\overset{\cdot(k)}{f_1} \\
&= \left(\frac{b_2c_2^k}{k!} + \bar{b}_2(1+\gamma)\frac{c_2^{k-1}}{(k-1)!} - \frac{1}{(k+1)!}\right) \\
&\quad \times\left(\overset{\cdot(k)}{f_1} - \mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - k\,\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}\,f_1^l\right) \\
&\quad + \left(\frac{\bar{b}_2c_2^{k-1}}{(k-1)!} - \frac{1}{(k+1)!}\right)\mathbf{f}_j\left(\overset{\cdot(k-1)}{f_1^j} - \mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l}\right) \\
&\quad + \left((k-1)\frac{\bar{b}_2c_2^{k-1}}{k!} - \frac{1}{(k+1)!}\right)k\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}\,f_1^l - \frac{1}{(k+1)!}\mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l} \\
&= \left(\frac{-k(k+1)c_2^2 + 2(k^2-1)c_2 - k(k-1)}{k(k-1)}\right) \\
&\quad \times\frac{1}{(k+1)!}\left(\overset{\cdot(k)}{f_1} - \mathbf{f}_j\overset{\cdot(k-1)}{f_1^j} - k\,\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}\,f_1^l\right) \\
&\quad + \frac{(k+1)c_2 - (k-1)}{k-1}\frac{1}{(k+1)!}\mathbf{f}_j\left(\overset{\cdot(k-1)}{f_1^j} - \mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l}\right) \\
&\quad + \frac{(k+1)c_2 - k}{k}\frac{k}{(k+1)!}\mathbf{f}_{jl}\overset{\cdot(k-2)}{f_1^j}\,f_1^l - \frac{1}{(k+1)!}\mathbf{f}_j\mathbf{f}_l^j\overset{\cdot(k-2)}{f_1^l}\,.
\end{aligned} \tag{29}$$

Therefore, we can define relative errors $r_1(c_2)$, $r_2(c_2)$, $r_3(c_2)$, $r_4(c_2)$ to the Taylor coefficients (20) as follows:

$$r_1(c_2) = \left|\frac{-k(k+1)c_2^2 + 2(k^2-1)c_2 - k(k-1)}{k(k-1)}\right| \tag{30}$$

$$r_2(c_2) = \left|\frac{(k+1)c_2 - (k-1)}{k-1}\right|$$

$$r_3(c_2) = \left|\frac{(k+1)c_2 - k}{k}\right|$$

$$r_4(c_2) = 1.$$

From (23), we get the following term as the coefficient of truncation error term of $(k-1)$-th order formula:

$$(31)\qquad \left(\hat{b}_2\frac{c_2^{k-1}}{(k-1)!} + \hat{\hat{b}}_2(1+\gamma)\frac{c_2^{k-2}}{(k-2)!} - \frac{1}{k!}\right)\left(\overset{\cdot(k-1)}{f_1} - \mathbf{f}_j\ \overset{\cdot(k-2)}{f_1^j}\right) + \left(\hat{\hat{b}}_2\frac{c_2^{k-2}}{(k-2)!} - \frac{1}{k!}\right)\mathbf{f}_j\ \overset{\cdot(k-2)}{f_1^j}$$
$$= \frac{kc_2 - (k-1)}{k-1}\left(1 - \frac{\hat{\hat{b}}_2}{\bar{b}_2}\right)\frac{1}{k!}\left(\overset{\cdot(k-1)}{f_1} - \mathbf{f}_j\ \overset{\cdot(k-2)}{f_1^j}\right) - \left(1 - \frac{\hat{\hat{b}}_2}{\bar{b}_2}\right)\frac{1}{k!}\mathbf{f}_j\ \overset{\cdot(k-2)}{f_1^j}\ .$$

Also, we can define relative errors $\hat{r_1}(c_2)$, $\hat{r_2}(c_2)$ to the Taylor coefficients (20)

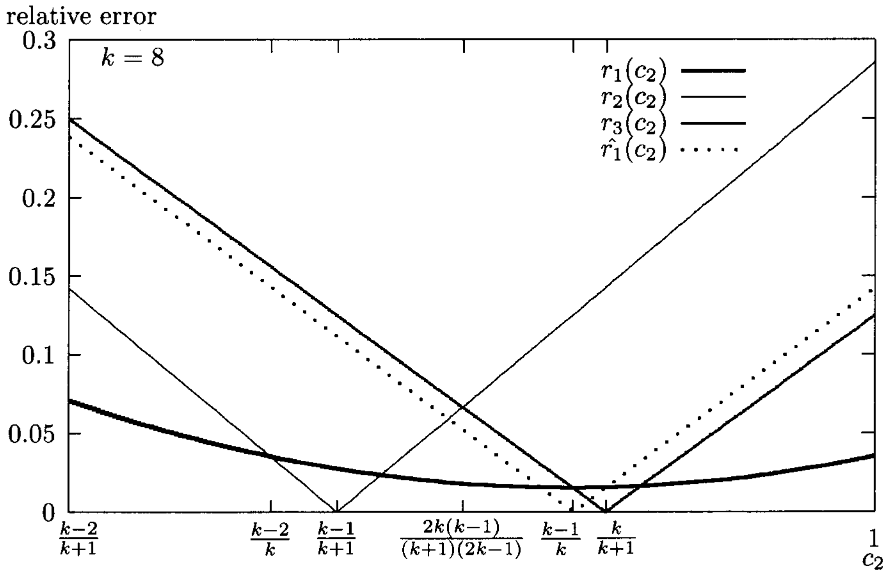

Fig. 1. Relative errors of h^k terms.

as follows:

$$\hat{r_1}(c_2) = \left| \frac{kc_2 - (k-1)}{k-1} \left(1 - \frac{\hat{\bar{b}}_2}{\bar{b}_2} \right) \right| \tag{32}$$

$$\hat{r_2}(c_2) = \left| \left(1 - \frac{\hat{\bar{b}}_2}{\bar{b}_2} \right) \right| \tag{33}$$

The relative errors $r_1(c_2)$, $r_2(c_2)$, $r_3(c_2)$ and $\hat{r_1}(c_2)$ for $k = 8$ as a function of c_2 are shown in Fig. 1.

2.5. Determination of free parameters

The stability region of our formula is independent of the value of free parameter c_2. Therefore we can not use the stability region to determine the value of c_2.

The formula (2) has special forms for $c_2 = \frac{k-2}{k}$ and $c_2 = \frac{k-1}{k}$.

If we choose $c_2 = \frac{k-2}{k}$, then the parameters b_2 and γ are zero from (25). Therefore $\tilde{f}_2$ becomes f_2 from (2). It follows that $\tilde{\dot{f}}_2$, the pseudo-derivative in the second stage, becomes the derivative as follows:

$$\tilde{\dot{f}}_2 = \left(\frac{\partial f}{\partial y} \right)_{y=y_{c_2}} \cdot f_2 = \dot{f}_2. \tag{34}$$

When $c_2 = \frac{k-1}{k}$, we can show from (25)–(28) that the parameters b_1, b_2 and $\overset{l}{\bar{b}_1}$ $(l = 1, 2, \ldots, k-3)$ of kth-order formula coincide with the parameters $\hat{b}_1$, $\hat{b}_2$ and $\overset{\hat{l}}{\bar{b}_1}$ $(l = 1, 2, \ldots, k-3)$ of $(k-1)$th-order formula respectively as follows:

$$b_1 = \hat{b}_1, \; b_2 = \hat{b}_2, \; \overset{(l)}{\bar{b}_1} = \overset{(\hat{l})}{\bar{b}_1} \quad (l = 1, 2, \ldots, k-3). \tag{35}$$

Hence, the estimation E of the truncation error of $\hat{y}_{n+1}$ becomes very simple:

$$E = h^2 \left(1 - \frac{\hat{\bar{b}}_2}{\bar{b}_2} \right) \tilde{\dot{f}}_2. \tag{36}$$

However, there is a greater probability that the error estimation E will be zero, because the relative error $\hat{r_1}(c_2)$ is zero from (32).

From Fig. 1, we see that the relative errors $r_1(c_2)$, $r_2(c_2)$, $r_3(c_2)$ decrease monotonously for $c_2 < \frac{k-1}{k+1}$, and increase monotonously for $\frac{k}{k+1} < c_2$. Therefore we choose c_2 from the interval $\left[\frac{k-1}{k+1}, \frac{k}{k+1}\right]$ except $c_2 = \frac{k-1}{k}$ in order to minimize the relative errors.

From the above discussions, we choose $c_2 = \frac{2k(k-1)}{(k+1)(2k-1)}$, where the lines $r_2(c_2)$ and $r_3(c_2)$ cross. For this c_2, the relative errors $r_1(c_2)$, $r_2(c_2)$ and $r_3(c_2)$ are less than $\frac{1}{2k-1}$, respectively.

3. Numerical Example and Conclusions

We will show that our derivations are correct by using a numerical example. That is to say, our formulas achieve definitely desired order of accuracy. We solve a system of equations [2]:

Integrate

$$\begin{aligned}
\frac{dy^{(1)}}{dt} &= y^{(2)}y^{(3)}, & y^{(1)}(0) &= 0,\\
\frac{dy^{(2)}}{dt} &= -y^{(1)}y^{(3)}, & y^{(2)}(0) &= 1,\\
\frac{dy^{(3)}}{dt} &= -k^2y^{(1)}y^{(2)}, & y^{(3)}(0) &= 1, \quad k^2 = 0.51
\end{aligned}$$

over the range $[0, 60]$. The errors in the numerical solution of $y(t)$ at $t = 60$ for various values of order k and of step size h by using the free parameter $c_2 = \frac{2k(k-1)}{(k+1)(2k-1)}$ are shown in Fig. 2. The computations were performed by IA-32 processor in

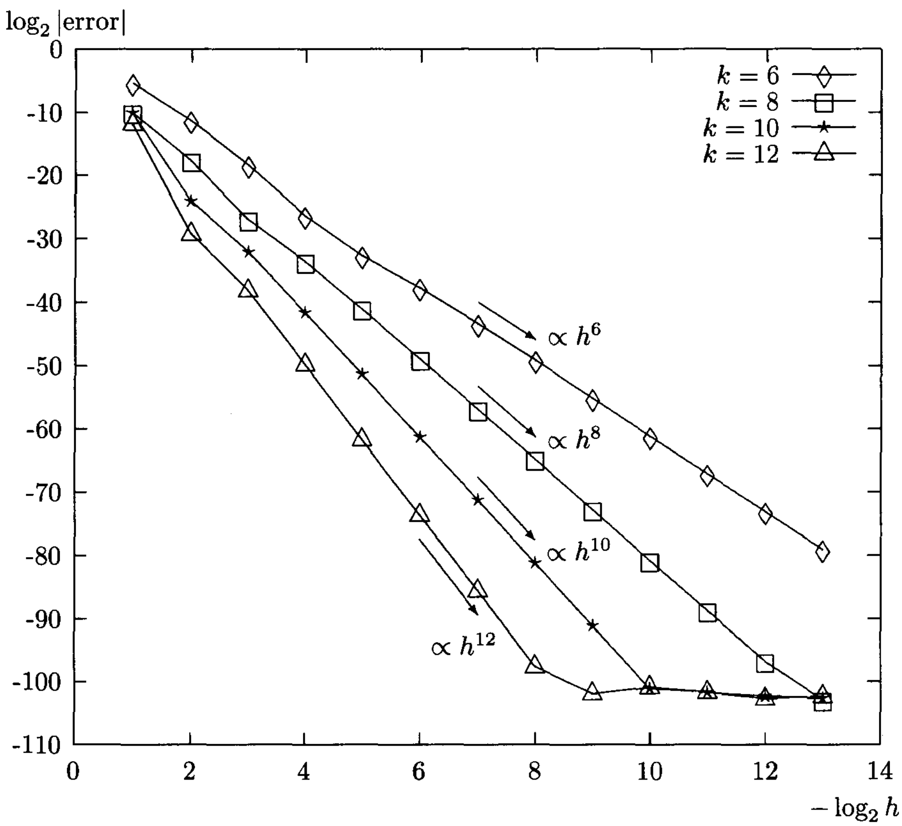

Fig. 2. Errors in numerical solution of $y(t)$ at $t = 60$.

quadruple-precision arithmetic (a normalized 113-bit fraction including the redundant most-significant fraction bit not represented), and NUMPAC[7] were used to calculate the true values in quadruple-precision arithmetic on hexadecimal system 28 figures.

From Fig. 2, we see that the proposed formula in general form achieves desired order.

The derivatives involved in our formula can be calculated very easily using the automatic differentiation. The proposed method has two clear advantages in computational cost. First, the higher derivatives $\overset{\cdot(i)}{f_1}$, $i = 1, 2, \ldots, m$ can be evaluated efficiently by using recursive computation of Taylor coefficients [4, 11]. The number of operations required for these derivatives is $O(m^2)$. Taylor series method of order k requires up to order $m = k-1$, however the proposed method requires up to order $m = k-3$. And secondly, the forward method of automatic differentiation computes the product of the Jacobian matrix $f_y(y)$ and a vector v without computing the Jacobian matrix itself [5, 11, 13]. The number of operations required to compute the product $f_y(y)v$ by this method is at most three times the number of operations required to compute $f(y)$. Since automatic methods for simultaneous computation of functions and their derivatives are now available [1, 6, 13], our formula will be one of the most promising methods.

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