# Five and Six Stage Runge-Kutta Type Formulas of Orders Numerically Five and Six

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New five- and six-stage Runge-Kutta type formulas of orders numerically five and six are proposed. It is well known that five and six stage explicit Runge-Kutta methods cannot achieve five and six order of accuracy. However, fifth- and sixth-order formulas are obtained when the distance between some pairs of abscissas tends to zero. Such formulas are called limiting formulas and involve derivatives. In previous papers we presented numerically fifth- and sixth-order formulas which require only five and six evaluations of the function. However, the parameters of these formulas are numbers of many decimal digits.

Parameters of our new formulas are simple, though our formulas can achieve the same accuracy as the limiting formulas. The values of derivatives in the limiting formulas do not require full significant digits carried in the computation. So, we approximate derivatives by numerical differentiation and choose one of free parameters of the limiting formula to minimize the error caused by approximation. As a result, the approximation errors in five- and six-stage formulas are reduced to $O(h^4r^{-q/2})$ and $O(h^3r^{-q/2})$ respectively with step size $h$ in $q$-digits of $r$ decimal system. Thus, the approximation errors are not a significant part of the total error throughout the computation.

## 1. Introduction

The system of ordinary differential equations considered has the form

$$dy/dt=f(t,y),\quad y(t_0)=y_0 \tag{1.1}$$

where $y$ and $f$ are vectors and the function $f$ is assumed to be differentiable many times if necessary. An explicit s-stage $p$-th order Runge-Kutta method for numerical solution at $t_{n+1}=t_n+h$ is defined by

$$y_{n+1}=y_n+h\sum_{i=1}^{s}\mu_i f_i \tag{1.2}$$

where

$$f_1=f(t_n,y_n)$$
$$f_i=f\left(t_n+\alpha_i h,\ y_n+h\sum_{j=1}^{i-1}\beta_{ij}f_j\right),\quad (i=2,\ldots,s)$$

The parameters $\alpha_i$'s, $\beta_{ij}$'s and $\mu_i$'s are determined so that the Taylor series for $y_{n+1}$ and for $y(t_n+h)$ agree through terms in $h^p$.

It is well known that $p\leqq s-1$ for $s=5,6,7$. But, five and six stage formulas can achieve fifth and sixth order of accuracy as limiting cases where the distance between some pairs of $\alpha_i$'s approaches zero [8], [5]. Such formulas are called the limiting formulas in which the derivatives of $f$ are involved as an inevitable result.

In two previous papers [9], [6]. We presented five and six stage formulas without derivatives of orders numerically five and six respectively. However, the coefficients of these formulas are fractional numbers of which numerators and denominators are the numbers of many decimal digits.

In this paper, new formulas of orders numerically five and six are proposed. They make use of only five and six evaluations of function and can achieve numerically the same accuracy as the fifth- and sixth-order limiting formulas respectively. Our new formulas are obtained by replacing the derivative of $f$ involved in the limiting formula by the simplest numerical differentiation. Because, in the limiting formulas, the values of derivatives do not require full significant digits carried in the computation and two free parameters are left. So we choose one of these free parameters so as to minimize the error caused by numerical differentiation, and choose the other one to minimize the local truncation error of the limiting formulas. The magnitudes of local truncation error of our new formulas are no more than 1.2 and 1.5 times as large as the best limiting formulas from the aspect of minimization of the local truncation error. The errors caused by the numerical differentiation are not significant compared with the truncation errors of our new formulas.

Our new formulas have three advantages. Their parameters are relatively simple, so they can easily be programmed. And they give the same accuracy as the limiting formulas without any additional work for evaluation of derivatives. Furthermore we can apply these formulas in various precision arithmetic system by changing the value used in the numerical differentiation.

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## 2. The Limiting Formulas

First we will briefly review previous works on the limiting formulas because our formulas are based on them [5], [8].

### 2.1 Fifth-order Formulas

The equations of condition for the Runge-Kutta coefficients, resulting from Taylor series expansion, are given up to the eighth order by Butcher in the condensed form [2].

The equations for the five stage fourth-order formula have the solution with seven free parameters. There are nine equations of condition of $O(h^5)$. And it is proved that all of these equations hold if and only if

Case 1) $\alpha_5=1$ and $\alpha_2 \to 0$ (free parameters: $\alpha_3$, $\alpha_4$)

or

Case 2) $\alpha_5=1$ and $\alpha_4 \to \alpha_5(=1)$

and (either $\alpha_3=2/5$ or $40\alpha_2\alpha_3-15(\alpha_2+\alpha_3)+6=0$)

(free parameter: $\alpha_2$).

Then the formulas are called limiting formulas, in which some values of derivatives are used instead of those of functions. The interval of absolute stability for any fifth-order limiting formula is $(-3.22, 0)$. This interval is independent of the choice of free parameters. So, it is desirable that the formula has the leading local truncation error as small as possible. Such formula is found in the Case 1) and is

$$
\text{(2.1-1)}\quad \left|\begin{array}{l}
f_1=f(t_n, y_n) \\
Df_2=\left(\dfrac{\partial}{\partial t}+f_1\dfrac{\partial}{\partial y}\right)f(t_n, y_n) \\
f_3=f(t_n+\alpha_3 h, y_n+h(b_{31}f_1+b_{32}hDf_2)) \\
f_4=f(t_n+\alpha_4 h, y_n+h(b_{41}f_1+b_{42}hDf_2+b_{43}f_3)) \\
f_5=f(t_n+h, y_n+h(b_{51}f_1+b_{52}hDf_2+b_{53}f_3+b_{54}f_4)) \\
y_{n+1}=y_n+h(m_1f_1+m_2hDf_2+m_3f_3+m_4f_4+m_5f_5)
\end{array}\right.
$$

where

$$
b_{i1}=\lim_{\alpha_2\to 0}(\beta_{i1}+\beta_{i2}),\quad b_{i2}=\lim_{\alpha_2\to 0}\beta_{i2}\alpha_2,\quad (i=3, 4, 5)
$$

$$
b_{ij}=\lim_{\alpha_2\to 0}\beta_{ij},\quad (i=4, j=3;\ i=5, j=3, 4)
$$

$$
m_1=\lim_{\alpha_2\to 0}(\mu_1+\mu_2),\quad m_2=\lim_{\alpha_2\to 0}\mu_2\alpha_2
$$

$$
m_i=\lim_{\alpha_2\to 0}\mu_i,\quad (i=3, 4, 5)
$$

The parameters are expressed rationally in terms of $\alpha_3$ and $\alpha_4$ as follows:

$$
\text{(2.1-2)}\quad \left|\begin{array}{l}
m_5=\dfrac{20\alpha_3\alpha_4-15(\alpha_3+\alpha_4)+12}{60(1-\alpha_3)(1-\alpha_4)},\quad m_4=\dfrac{3-5\alpha_3}{60\alpha_4^2(1-\alpha_4)(\alpha_4-\alpha_3)}, \\
m_3=\dfrac{5\alpha_4-3}{60\alpha_3^2(1-\alpha_3)(\alpha_4-\alpha_3)},\quad m_2=\dfrac{10\alpha_3\alpha_4-5(\alpha_3+\alpha_4)+3}{60\alpha_3\alpha_4}, \\
m_1=1-m_3-m_4-m_5 \\
b_{31}=\alpha_3,\ b_{32}=\alpha_3^2/2, \\
b_{43}=\dfrac{\alpha_4^2(\alpha_4-\alpha_3)}{\alpha_3^2(3-5\alpha_3)},\quad b_{42}=\alpha_4^2/2-b_{43}\alpha_3,\quad b_{41}=\alpha_4-b_{43}, \\
b_{54}=\dfrac{(1-\alpha_3)(1-\alpha_4)(3-5\alpha_3)}{\alpha_4^2(\alpha_4-\alpha_3)(20\alpha_3\alpha_4-15(\alpha_3+\alpha_4)+12)}, \\
b_{53}=\dfrac{1}{m_5}\left[\dfrac{5\alpha_4-3}{60\alpha_3^2(\alpha_4-\alpha_3)}-m_4b_{43}\right], \\
b_{52}=1/2-b_{53}\alpha_3-b_{54}\alpha_4,\quad b_{51}=1-b_{53}-b_{54}
\end{array}\right.
$$

Many methods are obtained for various choice of free parameters [8], and two methods are especially important. The first one corresponds to $\alpha_3=1/2$, $\alpha_4=5/9$, and is given below. The magnitude of the leading local truncation error is minimized.

[RKD53]

$$
\begin{aligned}
f_1 &= f(t_n, y_n) \\
Df_2 &= \left(\frac{\partial}{\partial t} + f_1 \frac{\partial}{\partial y}\right) f(t_n, y_n) \\
f_3 &= f\left(t_n + \frac{1}{2}h,\ y_n + h\left(\frac{1}{2}f_1 + \frac{1}{8}hDf_2\right)\right) \\
f_4 &= f\left(t_n + \frac{5}{9}h,\ y_n + h\left(\frac{305}{729}f_1 + \frac{125}{1458}hDf_2 + \frac{100}{729}f_3\right)\right) \\
f_5 &= f\left(t_n + h,\ y_n + h\left(\frac{359}{775}f_1 + \frac{7}{310}hDf_2 - \frac{100}{31}f_3 + \frac{2916}{775}f_4\right)\right) \\
y_{n+1} &= y_n + h\left(\frac{233}{750}f_1 + \frac{3}{100}hDf_2 - \frac{8}{15}f_3 + \frac{2187}{2000}f_4 + \frac{31}{240}f_5\right)
\end{aligned}
$$

The second one corresponds to $\alpha_3=(5-\sqrt{5})/10$, $\alpha_4=(5+\sqrt{5})/10$, and has certain valuable property considered later. It is

[RKD51]

$$
\begin{aligned}
f_1 &= f(t_n, y_n) \\
Df_2 &= \left(\frac{\partial}{\partial t} + f_1 \frac{\partial}{\partial y}\right) f(t_n, y_n) \\
f_3 &= f\left(t_n + \frac{5-\sqrt{5}}{10}h,\ y_n + h\left(\frac{5-\sqrt{5}}{10}f_1 + \frac{3-\sqrt{5}}{20}hDf_2\right)\right) \\
f_4 &= f\left(t_n + \frac{5+\sqrt{5}}{10}h,\ y_n + h\left(-\frac{5+3\sqrt{5}}{10}f_1 - \frac{3+\sqrt{5}}{20}hDf_2 + \frac{5+2\sqrt{5}}{5}f_3\right)\right) \\
f_5 &= f\left(t_n + h,\ y_n + h\left((1+2\sqrt{5})f_1 + \frac{\sqrt{5}}{2}hDf_2 - \frac{5+3\sqrt{5}}{2}f_3 + \frac{5-\sqrt{5}}{2}f_4\right)\right) \\
y_{n+1} &= y_n + h\left(\frac{1}{12}f_1 + \frac{5}{12}f_3 + \frac{5}{12}f_4 + \frac{1}{12}f_5\right)
\end{aligned}
$$

### 2.2 Sixth-order Formulas

The complete solutions of six stage fifth-order Runge-Kutta equations are given by Cassity [3]. He classified the solutions into six cases. The value of $\alpha_6$ is 1 except in one case, so we restrict ourselves in the case where $\alpha_6=1$.

There are 20 equations of condition for sixth-order formula. It is well known that no choice of the parameters with distinct abscissas $\alpha_i$'s can satisfy all of these equations. But when $\alpha_6=1$, if $\alpha_2 \to 0$ and $\alpha_5 \to \alpha_6(=1)$, all of them hold and we have two parameters $\alpha_3$ and $\alpha_4$ at our disposal [5].

Similar to (2.1-1) and (2.1-2), the limiting formula of order six is written using derivatives as follows:

(2.2-1)

$$
\begin{aligned}
f_1 &= f(t_n, y_n) \\
Df_2 &= \left(\frac{\partial}{\partial t} + f_1 \frac{\partial}{\partial y}\right) f(t_n, y_n) \\
f_3 &= f(t_n+\alpha_3 h,\ y_n + h(b_{31}f_1 + b_{32}hDf_2)) \\
f_4 &= f(t_n+\alpha_4 h,\ y_n + h(b_{41}f_1 + b_{42}hDf_2 + b_{43}f_3)) \\
y_p &= y_n + h(b_{61}f_1 + b_{62}hDf_2 + b_{63}f_3 + b_{64}f_4) \\
f_6 &= f(t_n+h,\ y_p) \\
Df_5 &= \frac{\partial}{\partial t}f(t_n+h, y_p) + \frac{\partial}{\partial y}f(t_n+h, y_p) \\
&\quad \times (b_{561}f_1 + b_{562}hDf_2 + b_{563}f_3 + b_{564}f_4 + b_{565}f_6) \\
y_{n+1} &= y_n + h(m_1f_1 + m_2hDf_2 + m_3f_3 + m_4f_4 + m_5hDf_5 + m_6f_6)
\end{aligned}
$$

where the parameters $b_{ij}$ $(i=3, 4, 6;\ j=1, 2, \ldots, i-1)$ and $m_i$ $(i=1, 2, 3, 4)$ are the same as those of the five stage method and

$$
m_5 = -\lim_{\substack{\alpha_2\to 0\\ \alpha_5\to 1}} \mu_5(1-\alpha_5), \quad m_6 = \lim_{\substack{\alpha_2\to 0\\ \alpha_5\to 1}} (\mu_5+\mu_6),
$$

$$b_{56j}=\lim_{\substack{\alpha_2\to 0\\ \alpha_5\to 1}}\frac{b_{6j}-b_{5j}}{1-\alpha_5},\quad (j=1,2,3,4);\quad b_{565}=\lim_{\substack{\alpha_2\to 0\\ \alpha_5\to 1}}\frac{b_{65}}{1-\alpha_5},$$

The parameters are expressed rationally in terms of $\alpha_3$ and $\alpha_4$ as follows:

$$\text{(2.2-2)}\quad \left|\begin{aligned}
&b_{31}=\alpha_3,\quad b_{32}=\alpha_3^2/2,\\
&b_{43}=\frac{\alpha_4^2(\alpha_4-\alpha_3)}{3\alpha_3^2(1-2\alpha_3)},\quad b_{42}=\alpha_4^2/2-b_{43}\alpha_3,\quad b_{41}=\alpha_4-b_{43},\\
&b_{64}=\frac{(1-\alpha_3)(1-\alpha_4)(1-2\alpha_3)}{2\alpha_4^2(\alpha_4-\alpha_3)(5\alpha_3\alpha_4-3(\alpha_3+\alpha_4)+2)},\\
&b_{63}=\frac{-(1-\alpha_3)(6\alpha_4^2-7\alpha_4-2\alpha_3+3)}{6\alpha_3^2(\alpha_4-\alpha_3)(5\alpha_3\alpha_4-3(\alpha_3+\alpha_4)+2)},\\
&b_{62}=1/2-b_{63}\alpha_3-b_{64}\alpha_4,\quad b_{61}=1-b_{63}-b_{64},\\
&m_1=\frac{\alpha_3\alpha_4(30\alpha_3\alpha_4-4(\alpha_3+\alpha_4)+4)-2(\alpha_3+\alpha_4)^2+\alpha_3+\alpha_4}{60\alpha_3^2\alpha_4^2},\\
&m_2=\frac{5\alpha_3\alpha_4-2(\alpha_3+\alpha_4)+1}{60\alpha_3\alpha_4},\quad m_3=\frac{2\alpha_4-1}{60\alpha_3^2(\alpha_4-\alpha_3)(1-\alpha_3)^2},\\
&m_4=\frac{-2\alpha_3+1}{60\alpha_4^2(\alpha_4-\alpha_3)(1-\alpha_4)^2},\quad m_5=\frac{-5\alpha_3\alpha_4+3(\alpha_3+\alpha_4)-2}{60(1-\alpha_3)(1-\alpha_4)},\\
&m_6=\frac{1}{60(1-\alpha_3)^2(1-\alpha_4)^2}\times[\alpha_3\alpha_4(30\alpha_3\alpha_4-56(\alpha_3+\alpha_4-1))+24(\alpha_3+\alpha_4)^2-45(\alpha_3+\alpha_4)+20]\\
&b_{564}=(m_4(1-\alpha_4)-m_6b_{64})/m_5,\\
&b_{563}=(m_3(1-\alpha_3)-m_4b_{43}-m_6b_{63})/m_5,\\
&b_{562}=2-b_{563}\alpha_3-b_{564}\alpha_4,\quad b_{561}=2-b_{563}-b_{564},\quad b_{565}=-1
\end{aligned}\right.$$

We choose free parameters so that the leading local truncation error term is minimized, since the interval of absolute stability is independent of the values of free parameters and is $(-3.55, 0)$. The most recommendable formula corresponds to $\alpha_3=3/7$, $\alpha_4=4/7$, and is given as follows [5]:

$$\text{[RKD6]}\quad \left|\begin{aligned}
&f_1=f(t_n,y_n)\\
&\quad Df_2=\left(\frac{\partial}{\partial t}+f_1\frac{\partial}{\partial y}\right)f(t_n,y_n)\\
&f_3=f\left(t_n+\frac{3}{7}h,\ y_n+h\left(\frac{3}{7}f_1+\frac{9}{98}hDf_2\right)\right)\\
&f_4=f\left(t_n+\frac{4}{7}h,\ y_n+h\left(-\frac{4}{189}f_1-\frac{40}{441}hDf_2+\frac{16}{27}f_3\right)\right)\\
&\quad y_p=y_n+h\left(\frac{2327}{2376}f_1+\frac{25}{99}hDf_2-\frac{490}{297}f_3+\frac{147}{88}f_4\right)\\
&f_6=f(t_n+h,y_p)\\
&\quad Df_5=\frac{\partial}{\partial t}f(t_n+h,y_p)+\frac{\partial}{\partial y}f(t_n+h,y_p)\times\left(\frac{317489}{34848}f_1+\frac{7817}{2904}hDf_2-\frac{51401}{2178}f_3+\frac{63847}{3872}f_4-f_6\right)\\
&y_{n+1}=y_n+h\left(\frac{1919}{8640}f_1+\frac{11}{720}hDf_2+\frac{2401}{8640}f_3+\frac{2401}{8640}f_4-\frac{11}{720}hDf_5+\frac{1919}{8640}f_6\right)
\end{aligned}\right.$$

Another choice of free parameters will be considered later.

## 3. New Methods Based on Limiting Formulas

In two previous papers [9], [6], five and six stage Runge-Kutta type formulas, without using the values of derivatives, were presented. They achieve numerically the same accuracy as the fifth- and sixth-order limiting formulas [RKD53] and [RKD6] respectively. However, their coefficients are the fractional numbers with numerators and denominators of many digits. So it is troublesome to input these coefficients. The new formulas in this paper are more recommendable because of their simple coefficients which are the same as those of the limiting formulas.

In our new formulas the derivative of $f$ is replaced by the simplest numerical differentiation. Two free parameters in the limiting formulas are chosen so that the error caused by the numerical differentiation is small enough compared with the local truncation error and does not affect the accuracy of the limiting formulas. Thus the new formulas can achieve numerically the same accuracy as the limiting formulas.

### 3.1 Five Stage Method

#### 3.1.1 Derivation of the Method

Computing

$$f_2=f(t_n+\varepsilon h,\ y_n+\varepsilon hf_1)$$

with some small value of $\varepsilon$, which will be determined later, we use

$$\hat{F}_2=\frac{f_2-f_1}{\varepsilon} \tag{3.1-1}$$

instead of the derivative $hDf_2$ in the limiting formula (2.1-1). This is because

$$\hat{F}_2=\frac{f_2-f_1}{\varepsilon}=hDf_2+\varepsilon\frac{h^2}{2}D^2f_2+\varepsilon^2\frac{h^3}{6}D^3f_2+O(\varepsilon^3h^4)$$

where

$$D^kf_2=\left(\frac{\partial}{\partial t}+f_1\frac{\partial}{\partial y}\right)^k f(t_n,y_n)$$

The truncation error and roundoff error in $E=\hat{F}_2-hDf_2$ are estimated as follows:

$$\text{truncation error:}\quad E_T(\varepsilon)=\varepsilon\frac{h^2}{2}|D^2f_2| \tag{3.1-2}$$

$$\text{roundoff error:}\quad E_R(\varepsilon)=2r^{-q}\frac{|f_1|}{\varepsilon} \tag{3.1-3}$$

($q$-digit to the base $r$)

From (3.1-2) and (3.1-3) we get the optimum $\varepsilon$ and $E$ as follows:

$$\varepsilon_{opt}=\frac{2}{h}r^{-q/2}\sqrt{\frac{|f_1|}{|D^2f_2|}} \tag{3.1-4}$$

$$E_{opt}=h\left[2r^{-q/2}\sqrt{|f_1D^2f_2|}+\frac{2}{3}r^{-q}\frac{|f_1D^3f_2|}{|D^2f_2|}+O(r^{-3q/2})\right] \tag{3.1-5}$$

By using (3.1-5), approximate values $\hat{f}_k$, $(k=3, 4, 5)$ of $f_k$ and $\hat{y}_{n+1}$ of $y_{n+1}$ are written as follows:

$$\begin{aligned}
\hat{f}_3&=f(t_n+\alpha_3h,\ y_n+h(b_{31}f_1+b_{32}\hat{F}_2))\\
&=f_3+hb_{32}E_{opt}f_{y_3}+O(h^4)\\
\hat{f}_4&=f(t_n+\alpha_4h,\ y_n+h(b_{41}f_1+b_{42}\hat{F}_2+b_{43}\hat{f}_3))\\
&=f_4+hb_{42}E_{opt}f_{y_4}+h^2b_{43}b_{32}E_{opt}f_{y_3}f_{y_4}+O(h^4)\\
\hat{f}_5&=f(t_n+\alpha_5h,\ y_n+h(b_{51}f_1+b_{52}\hat{F}_2+b_{53}\hat{f}_3+b_{54}\hat{f}_4))\\
&=f_5+hb_{52}E_{opt}f_{y_5}+h^2(b_{53}b_{32}f_{y_3}+b_{54}b_{42}f_{y_4})\\
&\quad\times E_{opt}f_{y_5}+O(h^4)
\end{aligned}$$

where $f_{y_3}$, $f_{y_4}$ and $f_{y_5}$ denote

$$\frac{\partial}{\partial y}f(t_n+\alpha_3h,\ y_n+h(b_{31}f_1+b_{32}hDf_2)),$$

$$\frac{\partial}{\partial y}f(t_n+\alpha_4h,\ y_n+h(b_{41}f_1+b_{42}hDf_2+b_{43}f_3)),$$

$$\frac{\partial}{\partial y}f(t_n+\alpha_5h,\ y_n+h(b_{51}f_1+b_{52}hDf_2+b_{53}f_3+b_{54}f_4))$$

respectively. Since $f_{y_3}$, $f_{y_4}$ and $f_{y_5}$ will have nearly the same magnitude as $f_y$, so setting them equal to $f_y$, we get

$$\begin{aligned}
\hat{y}_{n+1}&=y_n+h(m_1f_1+m_2\hat{F}_2+m_3\hat{f}_3+m_4\hat{f}_4+m_5\hat{f}_5)\\
&=y_{n+1}+hm_2E_{opt}+h^2(m_3b_{32}+m_4b_{42}+m_5b_{52})\\
&\quad\times E_{opt}f_y+h^3(m_4b_{43}b_{32}+m_5(b_{53}b_{32}+b_{54}b_{42}))\\
&\quad\times E_{opt}f_y^2+O(h^5)
\end{aligned}$$

From (2.1-2) we get

$$\left|\begin{aligned}
&m_3b_{32}+m_4b_{42}+m_5b_{52}=m_2=\frac{10\alpha_3\alpha_4-5(\alpha_3+\alpha_4)+3}{60\alpha_3\alpha_4}\\
&m_4b_{43}b_{32}+m_5(b_{53}b_{32}+b_{54}b_{42})=\frac{5\alpha_3-2}{120\alpha_3}
\end{aligned}\right. \tag{3.1-6}$$

Since $\alpha_4\neq 1$ $(=\alpha_5)$, we cannot choose $\alpha_3$ and $\alpha_4$ so that both of the equations in (3.1-6) hold. So, we will choose $\alpha_3$ and $\alpha_4$ so as to satisfy $m_2=0$, then the error involved in $\hat{y}_{n+1}$ caused by the numerical differentiation becomes $O(h^4)$ and can be estimated as

$$\begin{aligned}
E_y&=|\hat{y}_{n+1}-y_{n+1}|\\
&=h^4\frac{|5\alpha_3-2|}{|120\alpha_3|}[2r^{-q/2}\sqrt{|f_1D^2f_2|}f_y^2+O(r^{-q})]
\end{aligned}$$

On the accumulated error of our five stage formula, we must consider the following three factors:

i) accumulated leading local truncation error of the formula:

$$E_F=E_6h^5 \quad (E_6 \text{ depends on the function } f) \tag{3.1-7}$$

ii) accumulated roundoff error incurred in numerical differentiation:

$$(3.1\text{-}8)\qquad E_N = h^3 \frac{|5\alpha_3 - 2|}{|60\alpha_3|} r^{-q/2} \sqrt{|f_1 D^2 f_2|} f_y^2$$

iii) accumulated roundoff error included in the computation of one step:

$$(3.1\text{-}9)\qquad E_r = cr^{-q}h^{-1}, \quad (c \text{ is some constant})$$

As $h$ decreases, $E_F$ and $E_N$ decrease but $E_r$ increases. So, if $E_N < E_F$ for the values of $h$ such that $E_F > E_r$, then the formula can achieve numerically fifth order accuracy.

Though the magnitudes of $\sqrt{|f_1 D^2 f_2|} f_y^2$ and $c$ vary according to the function $f$, we assume they are nearly the same magnitude as unity. Setting $E_F = E_r$, we get

$$h = E_6^{-1/6} r^{-q/6}$$

For this value of $h$, solving $E_N < E_F$ for $E_6$, we get

$$(3.1\text{-}10)\qquad E_6 > |(5\alpha_3 - 2)/60\alpha_3|^{3/2} r^{-q/4}$$

The most preferable choice of $\alpha_3$ and $\alpha_4$, provided $m_2 = 0$, is $\alpha_3 = (5-\sqrt{5})/10$ and $\alpha_4 = (5+\sqrt{5})/10$ [8]. In this case, (3.1-10) becomes

$E_6 > 4.4_{10}-7$ (for 14 hexadecimal digits arithmetic)

$E_6 > 1.1_{10}-4$ (for 6 hexadecimal digits arithmetic)

Next, we will determine the value of $\varepsilon_{opt}$ (3.1-4) as a constant independent of the function $f$ because we cannot know a priori the magnitude of $\sqrt{|f_1/D^2 f_2|}$. The truncation error of numerical differentiation $E_T(\varepsilon)$ (3.1-2) is small for well conditioned $f$ and is large for ill conditioned $f$. So $\varepsilon_{opt}$ for well conditioned $f$ is larger than that for ill conditioned $f$. We determine $\varepsilon_{opt}$ on the larger side so that $E_N$ (3.1-8) should not dominate over $E_F$ (3.1-7) when $f$ is well conditioned. This is because the accumulated truncation error $E_F$ of well conditioned $f$ is also smaller than that of ill conditioned $f$. So, $\sqrt{|f_1/D^2 f_2|}$ is taken to be 4 on the bases of numerical experience. Then $\varepsilon_{opt}$ becomes

$$(3.1\text{-}11)\qquad \varepsilon = \frac{8}{h} r^{-q/2} = \begin{cases} 2^{-25}h^{-1} & \text{(for 14 hexadecimal digits arithmetic)} \\ 2^{-9}h^{-1} & \text{(for 6 hexadecimal digits arithmetic)} \end{cases}$$

Now, we get a five stage method of numerically fifth order. It will work well except for the special case where $E_6 \doteqdot 0$.

### 3.1.2 The Five Stage Formula of Numerically Fifth Order

The five stage formula of numerically fifth order is as follows, which we denote by [RKN5] [5].

$$[\text{RKN5}]\qquad \left|\begin{array}{l} f_1 = f(t_n, y_n) \\ f_2 = f(t_n + \varepsilon h, y_n + h\varepsilon f_1), \quad F_2 = \dfrac{f_2 - f_1}{\varepsilon} \\ f_3 = f\left(t_n + \dfrac{5-\sqrt{5}}{10} h, y_n + h\left(\dfrac{5-\sqrt{5}}{10} f_1 + \dfrac{3-\sqrt{5}}{20} F_2\right)\right) \\ f_4 = f\left(t_n + \dfrac{5+\sqrt{5}}{10} h, y_n + h\left(-\dfrac{5+3\sqrt{5}}{10} f_1 - \dfrac{3+\sqrt{5}}{20} F_2 + \dfrac{5+2\sqrt{5}}{5} f_3\right)\right) \\ f_5 = f\left(t_n + h, y_n + h\left((1+2\sqrt{5}) f_1 + \dfrac{\sqrt{5}}{2} F_2 - \dfrac{5+3\sqrt{5}}{2} f_3 + \dfrac{5-\sqrt{5}}{2} f_4\right)\right) \\ y_{n+1} = y_n + h\left(\dfrac{1}{12} f_1 + \dfrac{5}{12} f_3 + \dfrac{5}{12} f_4 + \dfrac{1}{12} f_5\right) \end{array}\right.$$

where

$$\varepsilon = \frac{8}{h} r^{-q/2} = \begin{cases} \dfrac{1}{33554432h} & \text{(for 14 hexadecimal digits arithmetic)} \\ \dfrac{1}{512h} & \text{(for 6 hexadecimal digits arithmetic)} \end{cases}$$

## 3.2 Six Stage Method

### 3.2.1 Derivation of the Method

We evaluate $\hat{F}_2$ in the same way as in the five stage method, and $\hat{F}_5$, which is used instead of the derivative $Df_5$ in the limiting formula (2.2-1), as follows. Computing

$$\hat{f}_5 = f(t_n + h - \delta h, y_n + h(b_{61} f_1 + b_{62}\hat{F}_2 + b_{63}\hat{f}_3 + b_{64}\hat{f}_4) - \delta h(b_{561} f_1 + b_{562}\hat{F}_2 + b_{563}\hat{f}_3 + b_{564}\hat{f}_4 + b_{565}\hat{f}_6))$$

we use

$$\hat{F}_5=\frac{\hat{f}_6-\hat{f}_5}{\delta}$$

instead of $hDf_5$ with some small value of $\delta$.

Next we will consider the error included in $\hat{F}_5$. Letting

$$\bar{f}=b_{561}f_1+b_{562}hDf_2+b_{563}f_3+b_{564}f_4+b_{565}f_6$$

and

$$D^kf_6=\left(\frac{\partial}{\partial t}+\bar{f}\frac{\partial}{\partial y}\right)^k f(t_n+h, y_p)$$

we can write $f_5$ as

$$f_5=f(t_n+h-\delta h, y_p-\delta h\bar{f})$$

$$=f_6-\delta hDf_6+\frac{\delta^2h^2}{2}D^2f_6+O(\delta^3h^3)$$

then we get

$$\frac{f_6-f_5}{\delta}=hDf_6-\delta\frac{h^2}{2}D^2f_6+O(\delta^2h^3)$$

In similar way as in 3.1.1, we get the optimum $\delta$ and $\Delta=(f_6-f_5)/\delta-hDf_6$ as follows:

(3.2-1) $$\delta_{opt}=\frac{2}{h}r^{-q/2}\sqrt{\frac{|f_6|}{|D^2f_6|}}$$

(3.2-2) $$\Delta_{opt}=-h[2r^{-q/2}\sqrt{|f_6D^2f_6|}+O(r^{-q})]$$

Since

$$\hat{f}_6=f_6+hb_{62}E_{opt}f_{y_6}+h^2(b_{63}b_{32}f_{y_3}+b_{64}b_{42}f_{y_4})E_{opt}f_{y_6}+O(h^4)$$

$$\begin{aligned}\hat{f}_5&=f(t_n+h-\delta h, y_p+hb_{62}E_{opt}+h^2(b_{63}b_{32}f_{y_3}+b_{64}b_{42}f_{y_4})E_{opt}-\delta h\bar{f}-\delta hb_{562}E_{opt}\\&\quad-\delta h^2(b_{563}b_{32}f_{y_3}+b_{564}b_{42}f_{y_4}+b_{565}b_{62}f_{y_6})E_{opt}+O(h^4))\\&=f_6-\delta hDf_6+hb_{62}E_{opt}f_{y_6}+h^2(b_{63}b_{32}f_{y_3}+b_{64}b_{42}f_{y_4})E_{opt}f_{y_6}-\delta hb_{562}E_{opt}f_{y_6}\\&\quad-\delta h^2(b_{563}b_{32}f_{y_3}+b_{564}b_{42}f_{y_4}+b_{565}b_{62}f_{y_6})E_{opt}f_{y_6}+O(h^4)\end{aligned}$$

we get

$$\hat{F}_5=\frac{\hat{f}_6-\hat{f}_5}{\delta_{opt}}=hDf_6+\Delta_{opt}+hb_{562}E_{opt}f_y+h^2(b_{563}b_{32}+b_{564}b_{42}+b_{565}b_{62})E_{opt}f_y^2+O(h^4)$$

From these values, we obtain

$$\begin{aligned}\hat{y}_{n+1}&=y_n+h(m_1f_1+m_2\hat{F}_2+m_3\hat{f}_3+m_4\hat{f}_4+m_5\hat{F}_5+m_6\hat{f}_6)\\&=y_{n+1}+h(m_2E_{opt}+m_5\Delta_{opt})+h^2(m_2b_{32}+m_4b_{42}+m_5b_{562}+m_6b_{62})E_{opt}f_y+O(h^4)\\&=y_{n+1}+h^22r^{-q/2}(m_2\sqrt{|f_1D^2f_2|}-m_5\sqrt{|f_6D^2f_6|})+h^2(m_2b_{32}+m_4b_{42}+m_5b_{562}+m_6b_{62})E_{opt}f_y+O(h^4)\end{aligned}$$

In this case, we can not choose $\alpha_3$ and $\alpha_4$ so that both of $m_2$ and $m_5$ vanish, because the numerator of $m_5$ is the factor of the denominator of $b_{6j}$'s. However, if we choose $\alpha_3$ and $\alpha_4$ so as to satisfy $m_2-m_5=0$, assuming both of the magnitudes of $\sqrt{|f_1D^2f_2|}$ and $\sqrt{|f_6D^2f_6|}$ are nearly equal, then the leading error term caused by numerical differentiation will become $O(h^3)$. From (2.2-2) we get

(3.2-3) $$m_2-m_5=\frac{(10\alpha_3^2-10\alpha_3+2)\alpha_4^2-(10\alpha_3^2-12\alpha_3+3)\alpha_4+2\alpha_3^2-3\alpha_3+1}{60\alpha_3\alpha_4(1-\alpha_3)(1-\alpha_4)}$$

(3.2-4) $$m_3b_{32}+m_4b_{42}+m_5b_{562}+m_6b_{62}=m_2=\frac{5\alpha_3\alpha_4-2(\alpha_3+\alpha_4)+1}{60\alpha_3\alpha_4}$$

The leading truncation error of the limiting formula consists of the sum of 48 terms. Their coefficients $\tau_{7,j}$ are divided into five classes as follows:
the multiples of

i) $$\xi=\frac{14\alpha_3\alpha_4-7(\alpha_3+\alpha_4)+4}{302400}$$ (13 terms)

ii) $$\eta=\frac{7\alpha_4-4}{15120}$$ (12 terms)

iii) $$\zeta=\frac{7\alpha_3-3}{15120}$$ (10 terms)

iv) $$\omega=\frac{1}{30240(1-2\alpha_3)(5\alpha_3\alpha_4-3(\alpha_3+\alpha_4)+2)^2}$$
$$\times[(305\alpha_4^2-296\alpha_4+72)\alpha_3^3+(175\alpha_4^3-466\alpha_4^2+340\alpha_4-76)\alpha_3^2$$

$$+(-210\alpha_4^3+395\alpha_4^2-248\alpha_4+52)\alpha_3+63\alpha_4^3-120\alpha_4^2+76\alpha_4-16] \qquad \text{(3 terms)}$$

v) $$K=\frac{1}{5040} \qquad \text{(10 terms)}$$

The magnitudes of $\sqrt{\Sigma\,\tau_{7,j}^2/48}$, $\max|\tau_{7,j}|$ and $|m_2|$ (coefficient of leading error term of numerical differentiation) are shown in Fig. 1, where $\alpha_4$ varies so as to satisfy $m_2-m_5=0$. In consideration of magnitude of local truncation error, we determine $\alpha_3=(5-\sqrt{10})/10$, $\alpha_4=\sqrt{10}/5$ so that the parameters are comparatively simple numbers of quadratic field. Then all of the parameters (2.2-2) are determined.

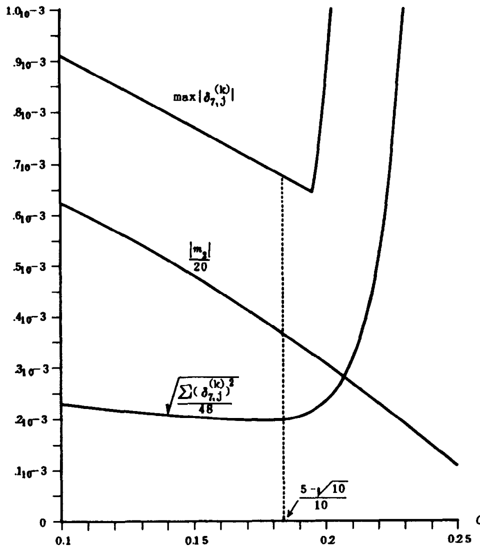


Fig. 1 magnitudes of the coefficient of leading truncation error term and approximation error

### 3.2.2 The Six Stage Formula of Numerically Sixth Order

Substituting $\alpha_3=(5-\sqrt{10})/10$ and $\alpha_4=\sqrt{10}/5$ into (2.2-2) and setting $\delta=\varepsilon$, we get six-stage formula of numerically sixth order [RKN6] [5].

[RKN6]

$$f_1=f(t_n, y_n)$$

$$f_2=f(t_n+\varepsilon h, y_n+h\varepsilon f_1), \quad F_2=\frac{f_2-f_1}{\varepsilon}$$

$$f_3=f\left(t_n+\frac{5-\sqrt{10}}{10}h,\ y_n+h\left(\frac{5-\sqrt{10}}{10}f_1+\frac{7-2\sqrt{10}}{40}F_2\right)\right)$$

$$f_4=f\left(t_n+\frac{\sqrt{10}}{5}h,\quad y_n+h\left(-\frac{220+23\sqrt{10}}{135}f_1-\frac{11+\sqrt{10}}{45}F_2+\frac{44+10\sqrt{10}}{27}f_3\right)\right)$$

$$y_p=y_n+h\left(\frac{1064+313\sqrt{10}}{54}f_1+\frac{55+14\sqrt{10}}{18}F_2-\frac{7240+2264\sqrt{10}}{351}f_3+\frac{50+17\sqrt{10}}{26}f_4\right)$$

$$f_6=f(t_n+h, y_p)$$

$$f_5=f\left(t_n+h-\varepsilon h,\ y_p-\varepsilon h\left(\frac{3198+1006\sqrt{10}}{9}f_1+\frac{464+146\sqrt{10}}{9}F_2\right.\right.$$

$$\left.\left.-\frac{45060+14296\sqrt{10}}{117}f_3+\frac{1240+406\sqrt{10}}{39}f_4-f_6\right)\right)$$

$$F_5=\frac{f_6-f_5}{\varepsilon}$$

$$y_{n+1}=y_n+\frac{100-37\sqrt{10}}{540}f_1+\frac{5-2\sqrt{10}}{180}F_2+\frac{280-40\sqrt{10}}{351}f_3+\frac{310+95\sqrt{10}}{1404}f_4+\frac{5-2\sqrt{10}}{180}F_5+\frac{-55+31\sqrt{10}}{270}f_6$$

where

$$\varepsilon=\frac{8}{h}r^{-q/2}=\begin{cases}\frac{1}{33554432h} & \text{(for 14 hexadecimal digits arithmetic)}\\ \frac{1}{512h} & \text{(for 6 hexadecimal digits arithmetic)}\end{cases}$$

## 4. Numerical Example and Conclusion

To illustrate that our formulas achieve numerically the same accuracy as the limiting formulas, we present the results of an example [7] in Fig. 2 and Fig. 3.

**Example 1.** Integrate

$$dy/dt=e^t(y^3(t+1)+1)/(3y^2(6-te^t)),\quad y(0)=1$$

over the range [0, 1]. The computations were performed in double and quadruple precision arithmetic using $\varepsilon$ (3.1-11) for double precision arithmetic.

Observations of figure 2 are as follows:

(1) For the values of step size $h$ larger than $2^{-8}$, the accumulated local truncation error $E_F$ (3.1-7) of the formula [RKN5] is the significant part of the total error and is of $O(h^5)$.

(2) For the values of $h$ smaller than $2^{-8}$, the accumulated roundoff error $E_r$ (3.1-9) dominates and is of $O(r^{-q}h^{-1})$.

(3) The accumulated error $E_N$ (3.1-8) caused by the numerical differentiation is insignificant in double precision arithmetic for all values of $h$ and is of $O(h^3r^{-q/2})$ as shown by the results using quadruple precision arithmetic.

Thus, our new formula [RKN5] can achieve numerically the same accuracy as the fifth-order limiting formula [RKD51].

On the formula [RKN6], the same situation is ob-

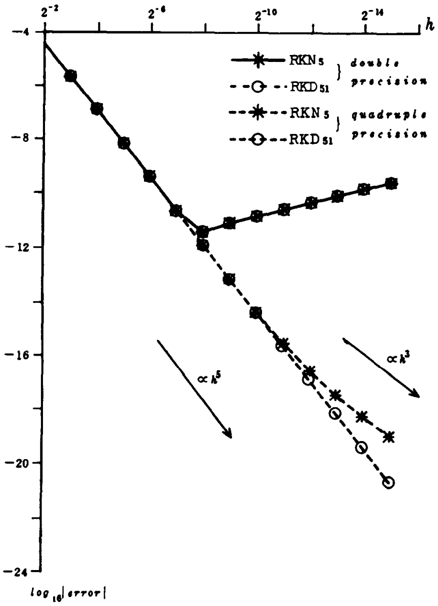


Fig. 2 Accumulated relative error of numerical solution of example 1) using [RKN5]

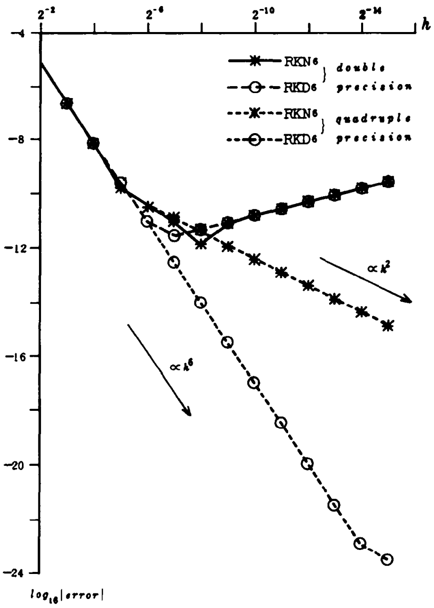


Fig. 3 Accumulated relative error of numerical solution of example 1) using [RKN6]

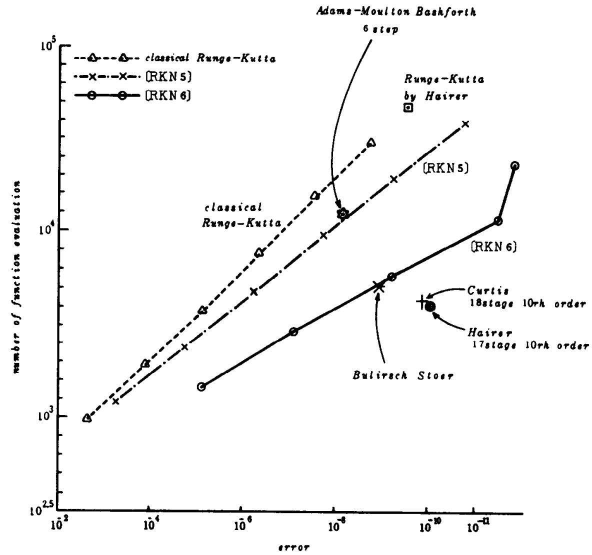


Fig. 4 Results of computation of Euler's equation

served in Fig. 3. However, in this case, $E_N$ is slightly larger than $E_F$ for $h=2^{-6}$ and $2^{-7}$, because $E_N$ is of $O(r^{-q/2}h^2)$ while $E_N$ in [RKN5] is of $O(r^{-q/2}h^3)$.

To compare the efficiency of our formula with other methods, we use the example in Bulirsch and Stoer [1] and in Hairer [4].

**Example 2.** Integrate Euler's equation of motion for a rigid body without external forces

$$dy_1/dt=y_2y_3, \quad y_1(0)=0$$
$$dy_2/dt=-y_1y_3, \quad y_2(0)=1$$
$$dy_3/dt=-k^2y_1y_2, \quad y_3(0)=1, \quad k^2=0.51$$

over the range [0, 60].

Figure 4 is the graph of the relation between the maximum error in the last step and the number of function evaluations. From this figure we see that our formula [RKN5] can achieve almost the same accuracy as Adams-Moulton-Bashforth's six step method, and the formula [RKN6] as Bulirsch-Stoer's polynomial extrapolation formula.

In conclusion, we are able to say that the formulas [RKN5] and [RKN6] are numerically of orders five and six respectively. Furthermore, since the leading truncation errors are minimized, they are the most accurate formulas with five and six evaluations of function.

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