Short Note

An Addendum to the Previous Paper "Runge-Kutta Type Seventh-order Limiting Formula (1989)"

HARUMI ONO* and HIDEO TODA*

In our paper on the Runge-Kutta type seventh-order limiting formula, which appeared in Vol. 12 No. 3 of this issue, the following problem is raised: similar to the five- and six-stage formulas, is it possible to derive a seven-stage formula of numerically seventh-order? Here we present the answer to this problem.

1. Introduction

The Runge-Kutta type seventh-order limiting formula of order seven is given as follows [2]:

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

$$F_2=\frac{\partial}{\partial t}f(t_n, y_n)+f_1\frac{\partial}{\partial y}f(t_n, y_n)$$

$$F_3=\frac{\partial^2}{\partial t^2}f(t_n, y_n)+2f_1\frac{\partial^2}{\partial t\,\partial y}f(t_n, y_n)+f_1^2\frac{\partial^2}{\partial y^2}f(t_n, y_n)+F_2\frac{\partial}{\partial y}f(t_n, y_n)$$

$$f_4=f\left(t_n+\alpha_4 h, y_n+h\left(b_{41}f_1+hb_{42}F_2+\frac{h^2}{2}b_{43}F_3\right)\right)$$

$$f_5=f\left(t_n+\alpha_5 h, y_n+h\left(b_{51}f_1+hb_{52}F_2+\frac{h^2}{2}b_{53}F_3+b_{54}f_4\right)\right)$$

$$y_p=y_n+h\left(b_{71}f_1+hb_{72}F_2+\frac{h^2}{2}b_{73}F_3+b_{74}f_4+b_{75}f_5\right)$$

$$f_7=f(t_n+h, y_p)$$

$$F_6=\frac{\partial}{\partial t}f(t_n+h, y_p)+\frac{\partial}{\partial y}f(t_n+h, y_p)\times\left(b_{671}f_1+hb_{672}F_2+\frac{h^2}{2}b_{673}F_3+b_{674}f_4+b_{675}f_5+b_{676}f_7\right)$$

$$y_{n+1}=y_n+h\left(m_1f_1+hm_2F_2+\frac{h^2}{2}m_3F_3+m_4f_4+m_5f_5+hm_6F_6+m_7f_7\right) \qquad (1.1)$$

where h is the step size, and the b_{ij}'s, b_{67j}'s and m_j's are the parameters which are expressed rationally in terms of two free parameters α_4 and α_5.

The problem is as follows: suppose that we replace F_2, F_3 and F_6 by the numerical differentiation and choose the values of free parameters so that the error caused by the approximation becomes as small as possible. Then, is the error caused by the numerical differentiation insifnificant compared with the truncation error of the formula (1.1)?

The results are summarized in the following table where the computation is done in q-digits of an r decimal system.

case	numerical differentiation	true derivative	local error caused by numerical differentiation
I	F_2, F_3, F_6	—	$O(h^6)$ (fifth-order formula)
II	F_3, F_6	F_2	$O(h^2r^{-q/2})$ (considerably large)
III	F_3	F_2, F_6	$O(h^6r^{-q/3})$ (small enough)

From this table we see that only the second derivative F_3 required in the limiting formula can be replaced by the numerical differentiation without loss of significance (case III).

2. Derivation of the Results

2.1 Case I

Computing f_2 as usual with some small value of ε and expanding it around the point (t_n, y_n), we get

$$f_2=f(t_n+\varepsilon h, y_n+\varepsilon hf_1)$$
$$=f_1+\varepsilon hDf+\frac{\varepsilon^2}{2}h^2D^2f+\frac{\varepsilon^3}{6}h^3D^3f+\ldots$$

where

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

We compute the numerical differentiation K_2 and then $\bar{f}_3$ using ε and K_2. K_2 and $\bar{f}_3$ can be expanded as follows:

$$K_2=\frac{f_2-f_1}{\varepsilon}=hDf+\frac{\varepsilon}{2}h^2D^2f+\frac{\varepsilon^2}{6}h^3D^3f+\ldots$$

*Faculty of Engineering, Chiba University.

$$\bar{f}_3=f\left(t_n+2\varepsilon h,\ y_n+2\varepsilon hf_1+\frac{(2\varepsilon)^2}{2}hK_2\right)$$
$$=f_1+2\varepsilon hDf+\frac{(2\varepsilon)^2}{2}h^2(Dff_y+D^2f)$$
$$+\frac{(2\varepsilon)^2}{2}h^3\left(\frac{\varepsilon}{2}D^2ff_y+2\varepsilon Df\,Df_y\right)$$
$$+\frac{(2\varepsilon)^3}{6}h^3D^3f+\ \dots$$

Using f_1, f_2 and $\bar{f}_3$, we get the numerical differentiation K_3,

$$K_3=\frac{\bar{f}_3-2f_2+f_1}{(2\varepsilon)^2}=\frac{1}{2}h^2(Dff_y+D^2f)-\frac{1}{4}h^2D^2f$$
$$+\frac{\varepsilon}{24}h^3(6D^2ff_y+24Df\,Df_y+7D^3f)+\ \dots$$

If we determine the value of ε optimal,

$$\varepsilon=\frac{2}{h}r^{-q/2}\sqrt{\frac{|f_1|}{|D^2f|}},\quad (q\text{-digits to the base } r)$$

then K_2 and K_3 can be written as follows:

$$K_2\fallingdotseq hF_2+hr^{-q/2}E_2,\quad (E_2=2\sqrt{|f_1D^2f|})$$
$$K_3\fallingdotseq\frac{h^2}{2}F_3-\frac{1}{4}h^2D^2f+h^2r^{-q/2}E_3,$$
$$\left(E_3=\frac{1}{12}\sqrt{\frac{|f_1|}{|D^2f|}}(6D^2ff_y+24Df\,Df_y+7D^3f)\right)$$

In the same way, we replace F_6 by the numerical differentiation $K_6=(\bar{f}_7-\bar{f}_6)/\varepsilon$ using

$$\bar{f}_6=f(t_n+(1-\varepsilon)h,$$
$$\bar{y}_p-\varepsilon h(b_{671}f_1+b_{672}K_2+b_{673}K_3+b_{674}\bar{f}_4$$
$$+b_{675}\bar{f}_5+b_{676}\bar{f}_7))$$

where the symbol $-$ is used to denote the value obtained by use of K_2 and K_3. As a result, we obtain $\bar{y}_{n+1}$ as follows:

$$\bar{y}_{n+1}\fallingdotseq y_n-\frac{h^3}{4}m_3D^2f-\frac{h^4}{4}m_3D^2ff_y-\frac{h^5}{8}m_3D^2ff_y^2$$
$$-\frac{7\alpha_4-3}{10080\alpha_4}h^6D^2ff_y^3-\frac{1}{10080}h^7D^2ff_y^4$$
$$+O(h^8)$$
$$+r^{-q/2}\left\{h^2(m_2E_2-m_6E_6)\right.$$
$$+h^3\left(m_3E_3+\left(m_2-\frac{3}{2}m_3\right)E_2f_y\right)$$
$$+h^4(m_3E_3f_y+(m_2-2m_3)E_2f_y^2)$$
$$\left.+O(h^5)\right\}\qquad(2.1)$$

In order to achieve numerically seventh order, at least all the terms which do not involve $r^{-q/2}$ must be zero. But it is impossible, because, provided $\alpha_5\neq 1(=\alpha_7)$, no choice of free parameters α_4 and α_5 satisfies both of the equations

$$m_3=\frac{14\alpha_4\alpha_5-7(\alpha_4+\alpha_5)+4}{420\alpha_4\alpha_5}=0$$

and

$$\frac{7\alpha_4-3}{10080\alpha_4}=0$$

Thus, the formula can achieve at most fifth order accuracy.

2.2 Case II

In this case we use the exact value of derivative F_2 and compute f_3 with some small value of δ. Since f_3 can be written

$$f_3=f\left(t_n+\delta h,\ y_n+\delta hf_1+\frac{\delta^2}{2}h_2Df\right)$$
$$=f_1+\delta hDf+\frac{\delta^2}{2}h^2(Dff_y+D^2f)$$
$$+\frac{\delta^3}{6}h^3(3Df\,Df_y+D^3f)+O(\delta^4h^4)$$

the numerical differentiation K_3 becomes

$$K_3=\frac{1}{\delta}\left\{\frac{f_3-f_1}{\delta}-hDf\right\}=\frac{h^2}{2}(Dff_y+D^2f)$$
$$+\frac{\delta}{6}h^3(3Df\,Df_y+D^3f)+O(\delta^2h^4)$$

If we choose the value of δ optimal, δ and K_3 become as follows:

$$\delta=\frac{1}{h}r^{-q/3}\sqrt[3]{24}\sqrt[3]{\frac{f_1}{3Df\,Df_y+D^3f}}$$
$$K_3\fallingdotseq\frac{h^2}{2}F_3+h^2r^{-q/3}E_3,$$
$$\left(E_3=\frac{2\sqrt[3]{3}}{3}\sqrt[3]{f_1(3Df\,Df_y+D^3f)^2}\right)$$

On the numerical differentiation $K_6=(\bar{f}_7-\bar{f}_6)/\delta'$, we get

$$\delta'=\frac{1}{h}r^{-q/2}\phi(f)$$
$$K_6\fallingdotseq hF_6+hr^{-q/2}E_6$$

where $\phi(f)$ and E_6 are the values that depend on the function f, Df, Df_y, . . . , E_3, ... Using these values, we obtain

$$\bar{y}_{n+1}=y_n+h^2r^{-q/2}m_6E_6$$
$$+h^3r^{-q/3}m_3E_3+h^4r^{-q/3}m_3E_3f_y$$
$$+h^5r^{-q/3}\frac{m_3}{2}E_3f_y^2$$
$$+h^6r^{-q/3}\frac{7\alpha_4-3}{2520\alpha_4}E_3f_y^3+\ \dots\qquad(2.2)$$

We cannot choose α_4 and α_5 so that m_6 vanishes, since

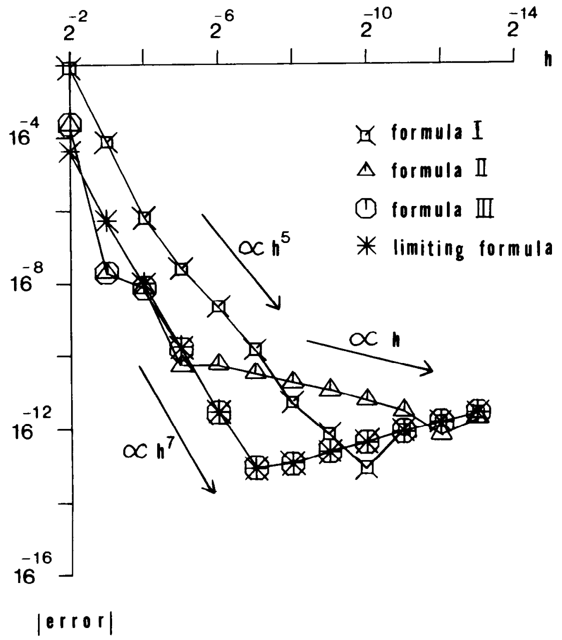

Fig. 1 The accumulated error of numerical solution in double precision arithmetic of the example using formulas I, II and III.

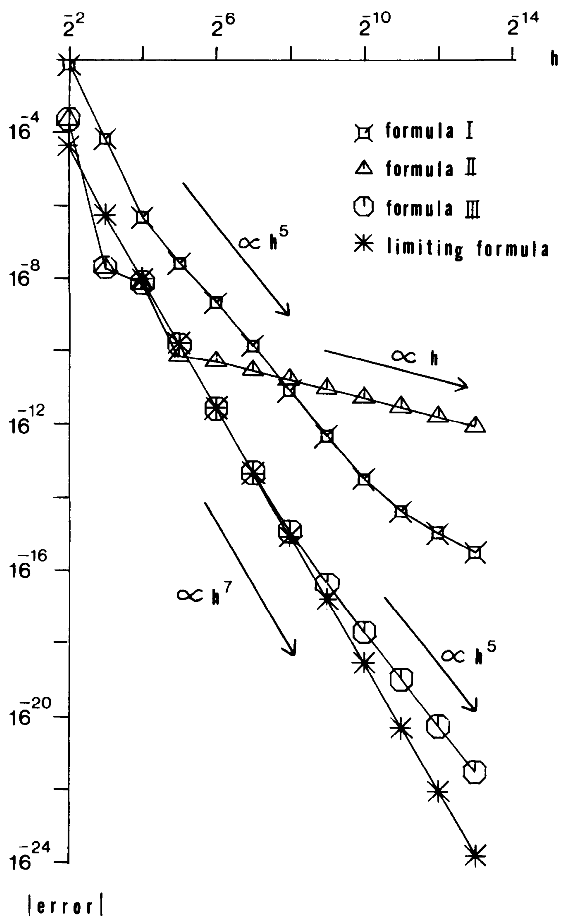

Fig. 2 The accumulated error of numerical solution in quadruple precision arithmetic of the example using formulas I, II and III with ε for double precision arithmetic.

m_6 is the factor of the denominators of the b_{67j}'s and b_{7j}'s. So the error caused by numerical differentiation becomes $O(h^2r^{-q/2})$. It is considerably large compared with the leading truncation error $O(h^8)$. Namely, this approximation error will overcome the truncation error of the limiting formula for comparatively large values of h by analogy with our argument in the previous paper [1] pp. 255–256.

2.3 Case III

If we use the derivative $\bar{F}_6(\fallingdotseq F_6)$, the second term of (2.2) $h^2r^{-q/2}m_6E_6$ will vanish. Then, if we choose α_4 and α_5 so that m_3 vanishes, it follows that the approximation error becomes $O(h^6r^{-q/3})$ and the formula can achieve numerically seventh order accuracy.

3. Numerical Example and Conclusions

In Fig. 1 and 2 we present the results of an example. Integrate

$$\frac{dy}{dt}=-\frac{t^2y^2}{3}, \qquad y(2)=1$$

over the range [2, 3] with varying step size h. The computations are performed in double and quadruple precision arithmetic using optimum ε for double precision arithmetic to illustrate the error caused by numerical differentiation.

The graphs indicate that

(1) Formula I (all of the derivatives, F_2, F_3 and F_6, are replaced by the numerical differentiation) is of order five (accumulated error is of $O(h^5)$) for all the value of h.

(2) Formula II (F_2 is derivative and F_3 and F_6 are replaced by the numerical differentiation) achieves the same accuracy as the limiting formula for the values of h larger than 2^{-5}, and for the values of h smaller than 2^{-5}, the accumulated error caused by the numerical differentiation becomes the significant part of the total error and is of $O(hr^{-q/2})$.

(3) Formula III (F_2 and F_6 are derivatives and F_3 is replaced by the numerical differentiation) achieves numerically the same accuracy as the limiting formula for all values of h and the accumulated error of the formula III caused by the numerical differentiation is of $O(h^5r^{-q/2})$ as shown by the results using quadruple precision arithmetic.

In conclusion, we see the following. In contrast to the five- and six-stage formulas, we cannot get a seven-stage formula of numerically seventh order by substituting numerical differentiations for all order derivatives required in the seventh order limiting formula. Only for the highest order derivative involved in the limiting formula, can we use numerical differentiation without loss of significance.

Acknowledgments

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References

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