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A FIFTH ORDER RUNGE-KUTTA RK(5, 5) METHOD WITH ERROR CONTROL

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In this paper a new Runge-Kutta RK(5, 5) method is introduced. The theory and analysis of its properties are investigated and compared with the more well known RKF(4, 5) and RK(4, 5) – Merson methods.

Keywords: Runge-Kutta methods; Error control; Arithmetic mean; Contraharmonic mean

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1 INTRODUCTION

In Evans and Yaakub [1], a new method called the RK(4, 4) was introduced using two different RK methods but of the same order p. The difference between these two approximations is taken to obtain an estimate of their accuracy. The RK(4, 4) method is based on the use of the fourth order classical Runge-Kutta method and the fourth order contraharmonic mean (C_oM) method (see Evans and Yaakub [1]). Now, we establish a new weighted RK(5, 5) strategy where we extend the RK(4, 4) method by using the fifth order RK methods. This approach is based on the use of the new fifth order arithmetic mean (AM) weighted Runge-Kutta method (Evans and Yaakub [2]) and the fifth order contraharmonic mean (C_oM) weighted Runge-Kutta method (Evans and Yaakub [1]). The combination of these two formula will be denoted as the RK(5, 5) method.

2 ERROR ESTIMATE OF RK(5, 5) METHOD

The combination of the fifth order arithmetic mean (AM) weighted Runge-Kutta formula

$$y_{\mathrm{AM}} = y_n + h\left[\sum_{i=1}^{4} w_i\left(\frac{k_i + k_{i+1}}{2}\right)\right] \tag{2.1}$$

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where $\sum_{i=1}^{4} w_i = 1$, $w_1 = 0.2615038147$, $w_2 = -0.2765809214$, $w_3 = 0.5947141647$, $w_4 = 0.4203629420$

$$\begin{aligned}
k_1 &= f(y_n) \\
k_2 &= f(y_n + 1.5471214403hk_1) \\
k_3 &= f(y_n + 0.1756458393hk_1 + 0.1243059001hk_2) \\
k_4 &= f(y_n + 0.1009316694hk_1 + 0.1100539630hk_2 + 0.2890143692hk_3) \\
k_5 &= f(y_n + 0.9997431862hk_1 - 0.0928890403hk_2 - 0.6201812828hk_3 \\
&\quad + 0.7133271396hk_4)
\end{aligned} \tag{2.2}$$

and the fifth order contraharmonic mean (C_oM) formula in the form

$$y_{C_oM} = y_n + h\left[\sum_{i=1}^{4} w_i\left(\frac{k_i^2 + k_{i+1}^2}{k_i + k_{i+1}}\right)\right] \tag{2.3}$$

where $\sum_{i=1}^{4} w_i = 1$, $w_1 = -0.1773157366$, $w_2 = 1.0254553152$, $w_3 = -0.0779114700$, $w_4 = 0.2297718914$

$$\begin{aligned}
k_1 &= f(y_n) \\
k_2 &= f(y_n + 0.1017275411hk_1) \\
k_3 &= f(y_n - 0.5236574475hk_1 + 1.1653361910hk_2) \\
k_4 &= f(y_n + 4.7450804540hk_1 - 4.2354437705hk_2 - 0.0096366835hk_3) \\
k_5 &= f(y_n - 0.5736403905hk_1 + 0.9301175162hk_2 + 0.4667978567hk_3 \\
&\quad + 0.1767250176hk_4)
\end{aligned} \tag{2.4}$$

is called RK(5, 5) method. The difference between Eq. (2.1) and (2.3), *i.e.*, $|y_{AM} - y_{C_oM}|$ provides an error estimate for the approximation to the numerical solution.

By using the same procedure as in the RK(4, 4) method, we can also obtain an error estimate for the five stage explicit AM $-$ C_oM method of order five by implementing the local truncation error for the fifth order arithmetic mean Runge-Kutta method and fifth order contraharmonic mean method.

For the fifth order arithmetic mean Runge-Kutta method, we have

$$y_{n+1}^{AM} = y_n + LTE^{AM} \tag{2.5}$$

and for the contraharmonic mean method

$$y_{n+1}^{C_oM} = y_n + LTE^{C_oM} \tag{2.6}$$

where y_{n+1}^{AM} and $y_{n+1}^{C_oM}$ are the numerical approximations at x_{n+1} obtained by the arithmetic mean and contraharmonic mean methods respectively and LTE^{AM} and LTE^{C_oM} are the local truncation errors of the fifth order arithmetic mean Runge-Kutta method and the fifth order contraharmonic mean methods.

An error estimate is obtained by taking the difference between these two methods for the numerical approximations at x_{n+1} by

$$y_{n+1}^{\mathrm{AM}} - y_{n+1}^{\mathrm{C_oM}} = LTE^{\mathrm{AM}} - LTE^{\mathrm{C_oM}} \tag{2.7}$$

The local truncation error for the fifth order arithmetic mean Runge-Kutta method involves y derivatives given by

$$\begin{aligned} LTE^{\mathrm{AM}} = h^6\Bigg[&\frac{1}{720} ff_y^5 + 0.0018022816 f^2 f_y^3 f_{yy} - 0.0166861138 f^3 f_y f_{yy}^2 \\ &+ 0.0082646021 f^3 f_y^2 f_{yyy} + 0.0041171137 f^4 f_{yy} f_{yyy} \\ &- 0.0023096163 f^4 f_y f_{yyyy} + 0.0000588245 f^5 f_{yyyyy} \Bigg] \ldots \end{aligned} \tag{2.8}$$

while the local truncation error for the contraharmonic mean method is given by

$$\begin{aligned} LTE^{\mathrm{C_oM}} = h^6[&0.0132485733 ff_y^5 + 0.0202501069 f^2 f_y^3 f_{yy} \\ &+ 0.0095106268 f^3 f_y f_{yy}^2 - 0.0022879188 f^3 f_y^2 f_{yyy} \\ &- 0.0001379536 f^4 f_{yy} f_{yyy} - 0.0003448339 f^4 f_y f_{yyyy} \\ &- 0.0000178190 f^5 f_{yyyyy}] \ldots \end{aligned} \tag{2.9}$$

The absolute difference between LTE^{AM} and $LTE^{\mathrm{C_oM}}$ is given by

$$\begin{aligned} \left| LTE^{\mathrm{AM}} - LTE^{\mathrm{C_oM}} \right| = h^6\Bigg[&\left(\frac{1}{720} - 0.0132485733 \right) ff_y^5 \\ &+ (0.0018022816 - 0.202501069) f^2 f_y^3 f_{yy} \\ &+ (-0.0166861138 - 0.0095106268) f^3 f_y f_{yy}^2 \\ &+ (0.0082646021 + 0.0022879188) f^3 f_y^2 f_{yyy} \\ &+ (0.0041171137 + 0.0001379536) f^4 f_{yy} f_{yyy} \\ &+ (-0.0023096163 + 0.0003448339) f^4 f_y f_{yyyy} \\ &+ (0.0000588245 + 0.0000178190) f^5 f_{yyyyy} \Bigg] \\ = h^6[&-0.0118597 ff_y^5 - 0.0184478 f^2 f_y^3 f_{yy} \\ &- 0.0261967 f^3 f_y f_{yy}^2 + 0.0105525 f^3 f_y^2 f_{yyy} \\ &+ 0.00425507 f^4 f_{yy} f_{yyy} - 0.00196478 f^4 f_y f_{yyyy} \\ &+ 0.0000766435 f^5 f_{yyyyy}] \ldots \end{aligned} \tag{2.10}$$

Following Lotkin [3], if the following bounds for f and its partial derivatives hold for $x \in [a,\ b]$ and $y \in [-\infty,\ \infty]$ we have,

$$\left|f(x,\ y)\right| < Q, \quad \left|\frac{\partial^{i+j} f(x,y)}{\partial x^i \partial y^j}\right| < \frac{P^{i+j}}{Q^{j-1}}, \quad i+j \leq p \tag{2.11}$$

where P and Q are positive constants and p is the order of the method. In this case, we have $p = 5$. Hence using (2.11), we have

$$\left.\begin{aligned} \left|ff_y^5\right| &< Q\left(\frac{P^{0+1}}{Q^{1-1}}\right)^5 \\ \left|f^2 f_y^3 f_{yy}\right| &< Q^2\left(\frac{P^1}{Q^0}\right)^3 \frac{P^2}{Q} \\ \left|f^3 f_y f_{yy}^2\right| &< Q^3 P\left(\frac{P^2}{Q}\right) \\ \left|f^3 f_y^2 f_{yyy}\right| &< Q^3 P^2\left(\frac{P^3}{Q^2}\right) \\ \left|f^4 f_{yy} f_{yyy}\right| &< Q^4 \frac{P^2}{Q}\cdot\frac{P^3}{Q^2} \\ \left|f^4 f_y f_{yyyy}\right| &< Q^4 P \frac{P^4}{Q^3} \\ \left|f^5 f_{yyyyy}\right| &< Q^5 \frac{P^5}{Q^4} \end{aligned}\right\} P^5 Q \ldots \tag{2.12}$$

From the Eqs. (2.9)–(2.12), we obtain

$$\left|LTE^{\mathrm{AM}} - LTE^{\mathrm{C_oM}}\right| \leq 0.0435848 P^5 Q h^6 \tag{2.13}$$

Hence,

$$\left|y_{n+1}^{\mathrm{AM}} - y_{n+1}^{\mathrm{C_oM}}\right| \leq 0.0435848 P^5 Q h^6 \tag{2.14}$$

or

$$\left|y_{n+1}^{\mathrm{AM}} - y_{n+1}^{\mathrm{C_oM}}\right| \leq \frac{89}{2042} P^5 Q h^6.$$

By taking the tolerence as TOL, *i.e.*, $\varepsilon < 0.00005$, then by setting

$$\left|y_{n+1}^{\mathrm{AM}} - y_{n+1}^{\mathrm{C_oM}}\right| \leq TOL$$

the error control and step size selection can be determined by (2.14) to give the formula as

$$0.0435848 P^5 Q h^6 < TOL$$

or

$$h < \left[\frac{TOL}{0.0435848P^5Q}\right]^{1/6} \tag{2.15}$$

3 EXPERIMENTAL RESULTS FOR RK(5, 5)

The following are the numerical results of testing the RK(5, 5) method for error control on the sample problems:

Problem 1 $y' + y = 0$
Initial condition: $x_0 = 0,\ y_0 = 1$
Exact solution: $y = \exp(-x)$

TABLE I

x	*Exact solution*	*Numerical solution*	*Absolute error*	*Estimate error*
$h = 0.50000$				
$h = 0.25000$				
$h = 0.50000$				
0.50000	0.6065104D + 00	0.6065307D + 00	0.2024324D − 04	0.1283099D − 04
1.00000	0.3678549D + 00	0.3678794D + 00	0.2455588D − 04	0.1556049D − 04
1.50000	0.2231078D + 00	0.2231302D + 00	0.2234047D − 04	0.1415296D − 04
2.00000	0.1353172D + 00	0.1353353D + 00	0.1806660D − 04	0.1144245D − 04
2.50000	0.8207130D − 01	0.8208500D − 01	0.1369721D − 04	0.8672849D − 05
3.00000	0.4977710D − 01	0.4978707D − 01	0.9969165D − 05	0.6310677D − 05
3.50000	0.3019033D − 01	0.3019738D − 01	0.7054254D − 05	0.4464323D − 05
4.00000	0.1831075D − 01	0.1831564D − 01	0.4889771D − 05	0.3093716D − 05
4.50000	0.1110566D − 01	0.1110900D − 01	0.3336465D − 05	0.2110405D − 05
5.00000	0.6735699D − 02	0.6737947D − 02	0.2248483D − 05	0.1421858D − 05
5.50000	0.4085271D − 02	0.4086771D − 02	0.1500126D − 05	0.9483790D − 06
6.00000	0.2477760D − 02	0.2478752D − 02	0.9925716D − 06	0.6273406D − 06
$h = 1.00000$				
7.00000	0.9085119D − 03	0.9118820D − 03	0.3370110D − 05	0.4554334D − 05
8.00000	0.3331210D − 03	0.3354626D − 03	0.2341614D − 05	0.3081334D − 05
9.00000	0.1221444D − 03	0.1234098D − 03	0.1265432D − 05	0.1590493D − 05
10.00000	0.4478627D − 04	0.4539993D − 04	0.6136600D − 06	0.7335390D − 06

The following is a list of sample problems used in the numerical experiments. The notation NPB defines the number of problem solution. The comparison of the time taken and accuracy between the RK(4, 4) (see Evans and Yaakub [1995]) and RKF(4, 5) methods are shown in Tables II and III.

Problem 2 (NPB 7) $y' + y - x - 1 = 0$
Initial conditions: $x_0 = 0,\ y_0 = 1$
Exact solution: $y = x + \exp(-x)$

Problem 3 (NPB 10) $y' - x^2\sin(x) + 1/x + 1 = 0$
Initial conditions: $x_0 = 1,\ y_0 = 4$
Exact solution: $y = -x - \log(x) + x^2\cos(x) - 2x\sin(x) - 2\cos(x) + C$

TABLE II

Problem	Time taken			
	RK(4, 4)	*RK4(5)-Merson*	*RKF(4, 5)*	*RK(5, 5)*
1	1.80	0.98	1.11	0.93
2	0.20	0.09	0.10	0.10
3	0.26	0.24	0.02	0.13
4	0.22	0.20	0.04	0.12
5	0.12	0.10	0.09	0.08

TABLE III

Problem	Absolute error			
	RK(4, 4)	*RK4(5)-Merson*	*RKF(4, 5)*	*RK(5, 5)*
1	0.2258×10^{-5}	0.2959×10^{-5}	0.1061×10^{-4}	0.6137×10^{-6}
2	0.8308×10^{-6}	0.1944×10^{-5}	0.2984×10^{-5}	0.6186×10^{-6}
3	0.3253×10^{-6}	0.3253×10^{-6}	0.1175×10^{-4}	0.2449×10^{-6}
4	0.2949×10^{-6}	0.6047×10^{-6}	0.2427×10^{-5}	0.5352×10^{-6}
5	0.5516×10^{-4}	0.1446×10^{-4}	0.7625×10^{-5}	0.3999×10^{-4}

Problem 4 (NPB 12) $y' + \ln(x^2) = 0$
Initial conditions: $x_0 = 1,\ y_0 = 2$
Exact solution: $y = -2(x \ln(x) - x)$

Problem 5 (NPB 4) $Y' - Y = 0$
Initial conditions: $x_0 = 0,\ y_0 = 1$
Exact solution: $y = \exp(x)$

In the new RK(5, 5) method with error control strategy, we use the error estimate as the difference between the fifth order AM Runge-Kutta method and the fifth order contraharmonic mean method. These error estimates ERREST used together with a constant derived in Eqs. (2.14)–(2.15) are in the form

$$\text{ERREST} = \left|Y_{\text{AM}} - Y_{\text{C}_o\text{M}}\right| \times \frac{89}{2042} \tag{3.1}$$

By using the error estimate in Eq. (3.1), the comparison of the time taken and the accuracy between solutions from the RK(5, 5), RK(4, 4), RKF (4, 5) and RK4(5)-Merson methods are shown in Table II and Table III.

From Table II, we can see that the solution for problems 1–5 by RK(5, 5) and RKF(4, 5) performed faster than the solution by Merson and RK(4, 4) methods. But in Table III, the accuracy for problems 1, 2, 3 and 4 of the RK(5, 5) is more accurate compared to RKF(4, 5), RK(4, 4) and Merson. However by reducing the step size to a certain value, *i.e.*, $h/2$ and $h/4$ the solution by the RK(5, 5), RK(4, 4), Merson and RKF(4, 5) methods are comparable in terms of the time taken and the accuracy.

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