

On Pseudo-Runge-Kutta Methods with 2 and 3 Stages

By

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§1. Introduction

In [3], Butcher has proved the following results for Runge-Kutta methods. Let $p^*(r)$ be the highest order that can be an r -stage method. Then

$$p^*(r) = r \quad (r = 1, 2, 3, 4),$$

$$p^*(5) = 4,$$

$$p^*(6) = 5,$$

$$p^*(7) = 6,$$

$$p^*(8) = 6,$$

$$p^*(9) = 7,$$

$$p^*(r) = r - 2 \quad (10 \leq r).$$

Pseudo-Runge-Kutta methods have been proposed by Byrne, Lambert and Costabile. We have seen in [1], [4] and [15] that Pseudo-Runge-Kutta methods have order

$$p^*(r) = r + 1 \quad (r = 2, 3, 4).$$

Byrne, Lambert and many other authors have shown that Pseudo-Runge-Kutta methods are less accurate than Runge-Kutta methods in the same order. In this paper, we shall present new Pseudo-Runge-Kutta methods which have order

$$p^*(r) = r + 2 \quad (r = 2, 3, 4).$$

In comparing our methods and other methods in the same order, our methods have almost the same accuracy as the Runge-Kutta type methods in order 5 and 6.

The outline of this paper is as follows: In Section 2, we present our new

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method. We see that there exists p -stage methods of order $p+2$ for $p=2, 3$.

We also discuss a choice of a free parameter of the methods.

In Section 3, we prove the convergence of the methods.

In Section 4, the local truncation error of the method is analysed. We give an estimate formula of the local truncation error.

In Section 5, we are concerned with systems of first order equations. In the last section, we present several numerical results. The results for 4-stage method of order 6 have been given in [7].

§2. Numerical Method

In this section, we discuss the initial value problem:

$$(2.1) \quad \begin{cases} y' = f(x, y) \\ y(x_0) = y_0 \end{cases} \quad (x, y) \in \Omega = \{(x, y); x_0 \leq x \leq x_0 + a, |y - y_0| \leq b\},$$

where $f(x, y)$ is assumed to be sufficiently smooth on Ω .

We introduce the following Pseudo-Runge-Kutta method:

$$(2.2) \quad \begin{aligned} y_{n+1} &= y_n + h\Phi(x_{n-1}, x_n, y_{n-1}, y_n; h), \\ \Phi(x_{n-1}, x_n, y_{n-1}, y_n; h) &= \sum_{i=0}^3 w_i k_i, \\ k_0 &= f(x_{n-1}, y_{n-1}), \quad k_1 = f(x_n, y_n), \\ k_2 &= f(x_n + a_2 h, y_n + b_0(y_n - y_{n-1}) + h \sum_{i=1}^2 b_i k_{i-1}), \\ k_3 &= f(x_n + a_3 h, y_n + c_0(y_n - y_{n-1}) + h \sum_{i=1}^3 c_i k_{i-1}), \\ a_2 &= \sum_{i=0}^2 b_i, \quad a_3 = \sum_{i=0}^3 c_i \quad (0 \leq a_2, a_3 \leq 1). \end{aligned}$$

In the above formula (2.2), the value y_n is to be an approximation to the value $y(x_n)$ of the solution of (2.1) for $x_n = x_0 + nh$.

The coefficients a_2, a_3, b_i ($i=0, 1, 2$) and c_i ($i=0, 1, 2, 3$) are real constants to be determined. The special case $b_0 = b_1 = c_0 = c_1 = w_0 = 0$ in (2.2) is Runge-Kutta method. The case $b_0 = c_0 = 0$ in (2.2) is due to Costabile [4].

We define the local truncation error $T(x_n, z(x_n); h)$ at x_n of the method (2.2) by

$$T(x_n, z(x_n), h) = z(x_{n+1}) - \{z(x_n) + h\Phi(x_{n-1}, x_n, z(x_{n-1}), z(x_n); h)\}.$$

where $z(x)$ is the solution of the initial value problem $z' = f(x, z), z(x_n) = y_n$.

Let D be the differential operator defined by

$$D = \frac{\partial}{\partial x} + f(x_n, y_n) \frac{\partial}{\partial y},$$

and put

$$\begin{aligned} D^i f(x_n, y_n) &= T^i \quad (i = 1, \dots, 5), \quad D^i f_y(x_n, y_n) = S^i \quad (i = 1, 2, 3), \\ (Df_y)^2(x_n, y_n) &= P, \quad (Df)^2(x_n, y_n) = Q, \quad Df_{yy}(x_n, y_n) = R, \\ f_y(x_n, y_n) &= f_y, \quad f_{yy}(x_n, y_n) = f_{yy}. \end{aligned}$$

We also introduce an abbreviation

$$\Sigma = \sum_{i=2}^3.$$

Assume that $y_n - z(x_n) = O(h^5)$. Then by the Taylor expansion about (x_n, y_n) , the formula (2.2) may be written as

$$\begin{aligned} y_{n+1} &= y_n + hA_1 k_1 + h^2 A_2 T + \frac{1}{2!} h^3 (A_3 f_y T + A_4 T^2) \\ &+ \frac{1}{3!} h^4 (B_1 T^3 + B_2 f_y T^2 + B_3 f_y^2 T + 3B_4 S T) + \frac{1}{4!} h^5 (C_1 T^4 \\ &+ 6C_2 T S^2 + 4C_3 T^2 S + 3C_4 f_{yy} Q + C_5 f_y T^3 + C_6 f_y^2 T^2 + C_7 f_y^3 T + C_8 f_y T S) \\ &+ \frac{1}{5!} h^6 (D_1 T^5 + D_2 T S^3 + D_3 T^2 S^2 + D_4 T^3 S + D_5 f_{yy} T^2 T + D_6 Q R \\ &+ D_7 T P + D_8 f_y T^4 + D_9 f_y^2 T^3 + D_{10} f_y^3 T^2 + D_{11} f_y^4 T + D_{12} f_{yy} f_y Q \\ &+ D_{13} f_y T S^2 + D_{14} f_y^2 T S + D_{15} f_y T^2 S) + O(h^7). \end{aligned}$$

The constants $\{A_i\}$, $\{B_i\}$, $\{C_i\}$ and $\{D_i\}$ are

$$\begin{aligned} A_1 &= w_0 + \sum_{i=1}^3 w_i, & A_2 &= -w_0 + \Sigma a_i w_i, \\ A_3 &= w_0 + \Sigma q_{1i} w_i, & A_4 &= w_0 + \Sigma a_i^2 w_i, \\ B_1 &= -w_0 + \Sigma a_i^3 w_i, & B_2 &= -w_0 + \Sigma q_{2i} w_i, \\ B_3 &= B_2 + g_1 w_3, & B_4 &= -w_0 + \Sigma a_i q_{1i} w_i, \\ C_1 &= w_0 + \Sigma a_i^4 w_i, & C_2 &= w_0 + \Sigma a_i^2 q_{1i} w_i, \\ C_3 &= w_0 + \Sigma a_i q_{2i} w_i, & C_4 &= w_0 + \Sigma q_{1i}^2 w_i, \\ C_5 &= w_0 + \Sigma q_{3i} w_i, & C_6 &= C_5 + g_2 w_i, \quad C_7 = C_6, \\ C_8 &= 3C_5 + 4C_3 + g_3 w_3, \\ D_1 &= -w_0 + \Sigma a_i^5 w_i, & D_2 &= 10(-w_0 + \Sigma a_i^3 q_{1i} w_i), \\ D_3 &= 10(-w_0 + \Sigma a_i^2 q_{2i} w_i), & D_4 &= 5(-w_0 + \Sigma a_i q_{3i} w_i), \\ D_5 &= 10(-w_0 + \Sigma q_{1i} q_{2i} w_i), & D_6 &= 15(-w_0 + \Sigma a_i q_{1i}^2 w_i), \end{aligned}$$

$$\begin{aligned}
 D_7 &= 3(D_4 + a_3 g_4 w_3), & D_8 &= (-w_0 + \sum q_4 i w_i), \\
 D_9 &= D_8 + g_5 w_3, & D_{10} &= D_9, \quad D_{11} = D_9, \\
 D_{12} &= D_5 + 3D_8 + g_6 w_3, & D_{13} &= D_3 + 6D_8 + g_7 w_3, \\
 D_{14} &= D_4 + 3D_9 + 4D_8 + g_8 w_3, \\
 D_{15} &= D_4 + 4D_8 + g_9 w_3,
 \end{aligned}$$

where

$$\begin{aligned}
 p_1 &= -b_0 - 2b_1, & p_2 &= b_0 + 3b_1, & p_3 &= -b_0 - 4b_1, \\
 p_4 &= b_0 + 5b_1, & p_5 &= -c_0 - 2c_1, & p_6 &= c_0 + 3c_1, \\
 p_7 &= -c_0 - 4c_1, & p_8 &= c_0 + 5c_1, \\
 q_{12} &= p_1, & q_{13} &= p_5 + 2a_2 c_3, & q_{22} &= p_2, & q_{23} &= p_6 + 3a_2^2 c_3, \\
 q_{32} &= p_3, & q_{33} &= p_7 + 4a_2^3 c_3, & q_{42} &= p_4, & q_{43} &= p_8 + 5a_2^4 c_3, \\
 g_1 &= 3c_3(p_1 - a_2^2), & g_2 &= 4c_3(p_2 - a_2^3), \\
 g_3 &= 12c_3(a_2 + a_3)(p_1 - a_2^2), & g_4 &= 20a_2 c_3(p_1 - a_2^2), \\
 g_5 &= 5c_3(p_3 - a_2^4), \\
 g_6 &= 15c_3((p_1 + a_2^2) + 2(p_5 + 2a_2 c_3))(p_1 - a_2^2), \\
 g_7 &= 30c_3(a_2^3 + a_2^2)(p_1 - a_2^2), & g_8 &= 20c_3(a_2 + a_3)(p_2 - a_2^3), \\
 g_9 &= 20c_3(a_2 + a_3)(p_2 - a_2^3).
 \end{aligned}$$

The method (2.1) is of order 5 if

$$\begin{aligned}
 (2.3) \quad A_1 &= 1, \quad A_2 = \frac{1}{2}, \quad A_3 = A_4 = \frac{1}{3}, \quad B_i = \frac{1}{4} \quad (i=1, \dots, 4), \\
 C_i &= \frac{1}{5} \quad (i=1, \dots, 8),
 \end{aligned}$$

and the condition (2.3) can be replaced by

$$\begin{aligned}
 (2.4) \quad A_1 &= 1, \quad A_2 = \frac{1}{2}, \quad A_4 = \frac{1}{3}, \quad B_1 = \frac{1}{4}, \quad C_1 = C_5 = \frac{1}{5}, \\
 a_2^2 &= p_1, \quad a_2^3 = p_2, \quad a_2^3 = p_5 + 2a_2 c_3, \quad a_3^3 = p_6 + 3a_2^2 c_3.
 \end{aligned}$$

From (2.4), we have

$$\begin{aligned}
 a_3 &= \frac{35a_2 - 27}{50a_2 - 35}, & w_3 &= \frac{10a_2 - 7}{12a_3(1 + a_3)(a_2 - a_3)}, \\
 w_2 &= \frac{5 - 6a_3(1 + a_3)w_3}{6a_2(1 + a_2)}, & w_0 &= a_2 w_2 + a_3 w_3 - \frac{1}{2}, \\
 w_1 &= 1 - (w_0 + w_2 + w_3), & b_0 &= -(3a_2^2 + 2a_2^3), \\
 b_1 &= -\frac{1}{2}(b_0 + a_2^2), & b_2 &= a_2 - (b_0 + b_1), \\
 c_3 &= \frac{1}{a_2 + 3a_2^2 + 2a_2^3} \left\{ \frac{1}{2} a_2^2 + a_2^3 + \frac{1}{10w_3} (1 - 5w_0 + 5(b_0 + 4b_1)w_2) \right\},
 \end{aligned}$$

$$c_0 = 6((a_2 + a_2^2)c_3 - \frac{1}{6}(3a_3^2 + 2a_3^3)),$$

$$c_1 = -\frac{1}{2}c_0 + a_2c_3 - \frac{1}{2}a_3^2, \quad c_2 = a_3 - (c_0 + c_1 + c_3).$$

The Optimal Method. If we assume that

$$|f(x, y)| \leq M,$$

$$\left| \frac{f^{i+j}(x, y)}{\partial x^i \partial y^j} \right| \leq L^{i+j} / M^{j-1} \quad (x, y) \in \Omega,$$

then we have

$$|T(x_n, z(x_n); h)| \leq CML^5h^6.$$

The constant C in the inequality is estimated by

$$(2.5) \quad 5!C \leq 32 \left| D_1 - \frac{1}{6} \right| + 8 \left| D_2 - \frac{4}{3} \right| + |D_2 + 4D_8 - 2| + 4 \left| D_3 - \frac{5}{3} \right|$$

$$+ \left| 2D_3 + 3D_4 - \frac{35}{6} \right| + \left| 4D_3 + 3D_4 - \frac{55}{6} \right| + \left| 2D_3 + D_4 - \frac{25}{6} \right|$$

$$+ \left| D_3 + 3D_4 - \frac{25}{6} \right| + \left| 2D_4 - \frac{5}{3} \right| + \left| D_5 - \frac{5}{6} \right| + 3 \left| D_5 + D_7 - \frac{25}{6} \right|$$

$$+ \left| D_3 + D_4 - \frac{15}{6} \right| + \left| 2D_5 + 2D_7 + 3D_{15} - \frac{77}{6} \right| + \left| D_5 + D_7 + D_{15} - \frac{17}{3} \right|$$

$$+ \left| D_7 + 2D_{15} - \frac{11}{2} \right| + \left| D_{12} - \frac{13}{6} \right| + |D_{13} - 2| + \left| D_{13} + 3D_9 - \frac{15}{6} \right|$$

$$+ |2D_{13} + 3D_9 + D_6 - 7| + \left| D_{13} + D_9 + D_6 - \frac{14}{3} \right| + |D_{14} - 2|$$

$$+ \left| D_8 - \frac{1}{6} \right| + \left| D_9 - \frac{1}{6} \right| + \left| D_{10} - \frac{1}{6} \right| + \left| D_{15} - \frac{3}{2} \right|$$

$$+ 2 \left| D_{13} + D_6 - \frac{9}{2} \right| + |D_{13} + 2D_6 - 7| + \left| D_{14} + 3D_{12} - \frac{19}{3} \right|$$

$$+ 2 \left| D_{11} - \frac{1}{6} \right| + 2 \left| D_6 - \frac{15}{6} \right| + \left| D_7 - \frac{15}{6} \right| + |6D_8 + 3D_2 - 5|$$

$$+ \left| 4D_8 + 3D_2 - \frac{14}{3} \right| + \left| D_8 + D_2 - \frac{3}{2} \right| + \left| 2D_{10} + D_{14} - \frac{7}{3} \right|$$

$$+ \left| D_{10} + D_{12} + D_{14} - \frac{13}{3} \right| + \left| D_{15} + D_5 - \frac{19}{6} \right| + \left| 2D_3 + 3D_4 - \frac{35}{6} \right|.$$

Let us denote the expression on the right hand side as $m(a_2)$.

We see that $m(a_2)$ is minimized if we set $a_2 = 0.4$, in which case the formula $I = \Upsilon(2.2)$ becomes

$$(2.6) \quad k_2 = f(x_n + 0.4h, 0.392y_n + 0.608y_{n-1} + 0.224hk_0 + 0.784hk_1),$$

$$k_3 = f(x_n + \frac{13}{15}h, \frac{1}{22754277}(60198640.32y_n - 37444363.32y_{n-1} - 13179377.12hk_0 - 39765362hk_1 + 35220749.2hk_2))$$

$$w_0 = \frac{-45.5}{107016}, \quad w_1 = \frac{14749}{107016}, \quad w_2 = \frac{56875}{107016}, \quad w_3 = \frac{35437.5}{107016},$$

and bound for C is

$$C = 0.52.$$

We compare the formula (2.6) with other methods of order 4 and 5. We shall present some numerical results in Table II.

These results also show that the formula (2.6) yields better results.

The method with $w_3 = 0$.

If we put $w_3 = 0$ in the formula (2.2), then it still gives 2-stages method of order 4. We may now proceed as in the case $w_3 \neq 0$.

The method (2.2) is of order 4 if

$$(2.7) \quad A_1 = 1, \quad A_2 = \frac{1}{2}, \quad A_3 = \frac{1}{3}, \quad B_1 = \frac{1}{4},$$

$$a_2^2 = p, \quad a_2^3 = p_5 + 2a_2c_3.$$

From (2.7) we have

$$(2.8) \quad k_2 = f(x + 0.7h, -1.156y_n + 2.156y_{n-1} + 0.833hf(x_{n-1}, y_{n-1}) + 2.023hf(x_n, y_n)),$$

$$w_0 = \frac{-7}{714}, \quad w_1 = \frac{221}{714}, \quad w_2 = \frac{500}{714}.$$

The local truncation error for this formula satisfies

$$|T(x_n, z(x_n); h)| \leq 1.33ML^4h^5.$$

Since the error bound is rather large, we compare this method with other method of order 3 by examples. These numerical results are given in Table I.

§3. Convergence of Our Method

In this section, we investigate the convergence of the method (2.2). Let e_n be defined by

$$e_n = y_n - y(x_n).$$

Theorem. *Let there exist constants $L > 0, N > 0$ and $p > 0$ such that*

$$(1) \quad |f(x, y_n) - f(x, y_{n-1})| \leq L|y_n - y_{n-1}| \quad (x, y_n), (x, y_{n-1}) \in \Omega,$$

$$(2) \quad |T(x_n, z(x_n); h)| \leq Nh^{p+1} \quad (x_n, y(x_n)) \in \Omega,$$

and let

$$\lim_{h \rightarrow 0} |e_1| = 0.$$

Then the method (2.2) is convergent.

Proof. From (1), we have

$$(3.1) \quad |\Phi(x_{n-1}, x_n, y_{n-1}, y_n; h) - \Phi(x_{n-1}, x_n, y(x_{n-1}), y(x_n); h)| \leq L(p_1|e_n| + p_2|e_{n-1}|),$$

where

$$p_1 = |w_1| + |w_2|(|1 + b_0| + hL|b_2|) + |w_3|(|1 + c_0| + hL(|c_2| + |c_3(1 + b_0)| + h^2L^2|c_3b_2|),$$

$$p_2 = |w_0| + |w_2|(|b_0| + hL|b_1|) + |w_3|(|c_0| + hL(|c_1| + |c_3b_0|) + h^2L^2|c_3b_1|).$$

Let us consider the following expression

$$(3.2) \quad y_{n+1} - y(x_{n+1}) = y_n - y(x_n) + h\Phi(x_{n-1}, x_n, y_{n-1}, y_n; h) - (y(x_{n+1}) - y(x_n)) = y_n - y(x_n) + h\Phi(x_{n-1}, x_n, y_{n-1}, y_n; h) - h\Phi(x_{n-1}, x_n, y(x_{n-1}), y(x_n); h) + h\Phi(x_{n-1}, x_n, y(x_{n-1}), y(x_n); h) - (y(x_{n+1}) - y(x_n)).$$

From (3.1) and (3.2), we have

$$|e_{n+1}| \leq (1 + hp_1L)|e_n| + hp_2L|e_{n-1}| + |T(x_n, z(x_n); h)|.$$

It follows that

$$|e_{n+1}| \leq \left(\sum_{j=1}^{n-1} T(x_j, z(x_j); h) + |e_1|\right)(1 + hL(p_1 + p_2))^n.$$

From (2) and the inequality $nh \leq a$, we have

$$|e_n| \leq (aNh^p + |e_1|) \exp(aL(p_1 + p_2)).$$

This shows that

$$\lim_{h \rightarrow 0} |e_n| = 0.$$

§ 4. Local Truncation Error Estimate

We represent the truncation error of the formula (2.2) in the form

$$T(x_n, z(x_n); h) = h^6\varphi(x_n, z(x_n)) + h^7\varphi_1(x_n, z(x_n)) + O(h^8).$$

Let $e(x)$, $v(x)$ and $e_1(x)$ be solutions of the following initial value problems.

$$\begin{cases} e' = ge - \varphi \\ e(x_0) = 0, \end{cases} \quad \begin{cases} v' = gv - b \\ v(x_0) = 0, \end{cases} \quad \begin{cases} e_1' = g_1 e_1 \\ e_1(x_0) = 1 \end{cases} \quad \text{respectively,}$$

where

$$\begin{aligned} e &= e(x), \quad v = v(x), \quad \varphi = \varphi(x, y(x)), \quad g = f_y(x, y(x)), \\ b &= \varphi(x, y(x)) - \left\{ a(x) - \frac{1}{2}(g(x)\varphi(x)) \right\} - \frac{1}{2} \varphi'(x), \\ a(x) &= \sum j \Phi_j(x, x, (x), \varphi(x); h), \quad \Phi_j = \frac{\partial}{\partial u_j}(x, x, u_1, u_2; h). \end{aligned}$$

Then the global error of the formula (2.2) is given by

$$(4.1) \quad e_n = h^5 e(x_n) + h^6 v(x_n) + h^6 A_1 e_1(x_n) + O(h^7) \quad (n = 1, 2, \dots),$$

where A_1 is a function of the starting value.

The detailed proof is given in [9].

Let us now consider the following difference equation:

$$(4.2) \quad E(x_{n+2}, y_{n+2}) = h \sum_{j=0}^5 b_j f(x_{n+j}, y_{n+j}) + \sum_{j=1}^5 a_j y_{n+j},$$

where the constants $\{a_j\}$ and $\{b_j\}$ are real solutions of the following equations.

$$(4.3) \quad \begin{aligned} q \sum_{j=0}^5 j^{q-1} b_j + \sum_{j=1}^5 j^q a_j &= 0 \quad (q = 1, 2, \dots, 6), \\ \sum_{j=1}^5 a_j &= 0, \quad \sum_{j=1}^5 j a_j = -1, \quad \sum_{j=1}^5 j^2 a_j = -3. \end{aligned}$$

Using $y_{n+j} = y(x_{n+j}) + e_{n+j}$ and expanding in powers of e_n , we have

$$(4.4) \quad \begin{aligned} E(x_{n+2}, y_{n+2}) &= h \sum_{j=0}^5 b_j f(x_{n+j}, y_{n+j}) + \sum_{j=1}^5 a_j y(x_{n+j}) \\ &\quad + \sum_{j=0}^5 b_j f_y(x_{n+j}, y(x_{n+j})) e_{n+j} + \sum_{j=1}^5 a_j e_{n+j} + O(h^7). \end{aligned}$$

Expanding (4.4) in powers of h and marking use of (4.1) and (4.2), we have

$$\begin{aligned} E(x_{n+2}, y_{n+2}) &= T(x_{n+2}, z(x_{n+2}); h) + O(h^7), \\ E(x_{n+2}, y(x_{n+2})) &= O(h^8). \end{aligned}$$

From (4.2) and (4.3) we have

$$(4.5) \quad \begin{aligned} E(x_{n+2}, y_{n+2}) &= \frac{h}{75600} (-459f(x_n, y_n) + 18684f(x_{n+1}, y_{n+1}) \\ &\quad + 66312f(x_{n+2}, y_{n+2}) + 2160f(x_{n+3}, y_{n+3})) \end{aligned}$$

$$\begin{aligned}
 & -11097f(x_{n+4}, y_{n+4}) + \frac{1}{4200}(2858.5y_{n+1} \\
 & - 239y_{n+2} - 3834y_{n+3} + 1151y_{n+4} + 63.5y_{n+5}).
 \end{aligned}$$

Thus the equation (4.5) is the estimation formula of the local truncation error of the equation (2.4). The numerical tests are given in Table III.

§ 5. Methods for Systems of Equations of the First Order

In this section, we consider the numerical methods of the initial value problem for a system of ordinary differential equations:

$$(5.1) \quad \begin{cases} Y' = F(Y) & Y \in \Omega, \\ Y(a) = Y_0, \end{cases}$$

The formula we seek is the form

$$\begin{aligned}
 Y_{n+1} &= Y_n + h\Phi(Y_{n-1}, Y_n; h), \\
 \Phi(Y_{n-1}, Y_n; h) &= \sum_{i=0}^3 W_i K_i, \\
 K_0 &= F(Y_{n-1}), \quad K_1 = F(Y_n), \\
 K_2 &= F(Y_n + q_0(Y_n - Y_{n-1}) + h(q_1 - q_2)K_1 + hq_2K_0), \\
 K_3 &= F(Y_n + q_3(Y_n - Y_{n-1}) + h(q_4 - q_5 - q_6)K_1 + hq_5K_0 + hq_6K_2).
 \end{aligned}$$

In the above formula (5.2), the value Y_n is to be an approximation to the value $Y(x_n)$ of the solution of (5.1) for $x_n = a + nh$.

The coefficients W_i ($i=0, 1, 2, 3$) and q_i ($i=0, \dots, 6$) are real constants to be determined.

Using the same notation as in Henrici [6], Taylor expansion for (5.2) is

$$\begin{aligned}
 (5.3) \quad Y_{n+1} &= Y_n + h\tilde{A}_1 K_1 + h^2 \tilde{A}_2 B + \frac{1}{2!} h^3 \{ \tilde{A}_3 D + \tilde{A}_4 C \} + \frac{1}{3!} h^4 \{ \tilde{B}_1 E + \tilde{B}_2 G \\
 & + \tilde{B}_3 H + 3\tilde{B}_4 F \} + \frac{1}{4!} h^5 \{ \tilde{C}_1 I + 6\tilde{C}_2 J + 4\tilde{C}_3 K + 3\tilde{C}_4 R + \tilde{C}_5 M \\
 & + 3\tilde{C}_6 N + \tilde{C}_7 P + \tilde{C}_8 Q + 4\tilde{C}_9 L \} + \frac{1}{5!} h^6 \{ \tilde{D}_1 f_{ijklm} A^i A^j A^k A^l A^m \\
 & + \tilde{D}_2 f_{ijkl} A^i A^j A^k B^l + \tilde{D}_3 f_{ijk} A^i A^j C^k + \tilde{D}_4 f_{ij} A^i E^j + \tilde{D}_5 f_{ij} B^i C^j \\
 & + \tilde{D}_6 f_{ijk} A^i B^j B^k + \tilde{D}_7 f_{ij} A^i F^j + \tilde{D}_8 f_i I^i + \tilde{D}_9 f_i M^i + \tilde{D}_{10} f_i P^i \\
 & + \tilde{D}_{11} f_i Q^i + \tilde{D}_{12} f_{ij} A^i H^j + \tilde{D}_{13} f_{ij} B^i D^j + \tilde{D}_{14} f_{ijk} A^i A^j D^k \\
 & + \tilde{D}_{15} f_{ij} A^i G^j + \tilde{D}_{16} f_j K^i + \tilde{D}_{17} f_i N^i + \tilde{D}_{18} f_i R^i + \tilde{D}_{19} f_i L^i \\
 & + \tilde{D}_{20} f_i J^i \} + O(h^7).
 \end{aligned}$$

We may try to express the constants $\{\tilde{A}_i\}$, $\{\tilde{B}_i\}$, $\{\tilde{C}_i\}$ and $\{\tilde{D}_i\}$ by using the constants $\{A_i\}$, $\{B_i\}$, $\{C_i\}$ and $\{D_i\}$ in Section 2.

If we put

$$q_0 = b_0, q_1 = a_2 - b_0, q_2 = b_1, q_3 = c_0, q_4 = a_3 - c_0, q_5 = c_1, q_6 = c_3,$$

then we have

$$\begin{aligned} \tilde{A}_i &= A_i \quad (i = 1, 2, 3, 4), \\ \tilde{B}_i &= B_i \quad (i = 1, 2, 3, 4), \\ \tilde{C}_i &= C_i \quad (i = 1, 2, \dots, 5), \\ \tilde{C}_6 &= C_5 + \frac{4}{3}a_2g_1W_3, \quad \tilde{C}_7 = \tilde{C}_8 = C_6, \\ \tilde{C}_9 &= C_3 + a_3g_1W_3, \\ \tilde{D}_i &= D_i \quad (i = 1, 2, \dots, 11), \\ \tilde{D}_{13} &= D_5 + (p_5 + 2a_2c_3)g_1W_3, \\ \tilde{D}_{14} &= D_3 + 10a_3^2g_1W_3, \\ \tilde{D}_i &= \frac{1}{3}D_7 + 20a_3c_3(p_2 - a_2p_1)W_3 \quad (i = 12, 15), \\ \tilde{D}_{16} &= 4D_8 + 5a_2g_2W_3, \\ \tilde{D}_{17} &= 3D_9, \\ \tilde{D}_{18} &= 3D_8 + 5(p_1 + a_2^2)g_1W_3, \\ \tilde{D}_{19} &= D_{16}, \\ \tilde{D}_{20} &= 6D_8 + 10a_2g_1W_3. \end{aligned}$$

We may proceed as in Section 2. The method (5.2) is of order 5 if

$$(5.4) \quad \tilde{A}_1 = 1, \quad \tilde{A}_2 = \frac{1}{2}, \quad \tilde{A}_4 = \frac{1}{3}, \quad \tilde{B}_1 = \tilde{B}_2 = \frac{1}{4},$$

$$(q_0 + q_1)^2 = -(q_0 + 2q_2), \quad (q_3 + q_4)^2 = -(q_3 + 2q_5) + 2(q_0 + q_1)q_6.$$

From (5.4) we have

$$\begin{aligned} W_3 &= \frac{10r_1 - 7}{12r(r+1)(r_1 - r)}, \quad W_2 = \frac{1}{r_1(r_1 + 1)} \left(\frac{5}{6} - r(r+1)W_3 \right), \\ W_0 &= r_1W_2 + rW_3 - \frac{1}{2}, \quad W_1 = 1 - (W_0 + W_2 + W_3), \\ q_0 &= -(3r_1^2 + 2r_1^3), \quad q_1 = r_1 - q_0, \quad q_2 = -\frac{1}{2}(q_0 + r_1^2), \\ q_6 &= \frac{1}{r_1 + 3r_1^2 + 2r_1^3} \left\{ \frac{1}{2}r^2 + r^3 + \frac{1}{10W_3} (1 - 5W_0 + 5(q_0 + 4q_2)W_2) \right\}, \\ q_3 &= 6(r_1 + r_1^2)q_6 - (3r^2 + 2r^3), \quad q_4 = r - q_3, \\ q_5 &= -\frac{1}{2}q_3 + r_1q_6 - \frac{1}{2}r^2, \end{aligned}$$

where

$$r_1 = q_0 + q_1, \quad r = \frac{35r_1 - 27}{50r_1 - 37}.$$

The local truncation error for this method may be written as

$$\begin{aligned} T(Y_n; h) = & \hat{D}_1 f_{ijklm} A^i A^j A^k A^l A^m + \hat{D}_2 f_{ijkl} A^i A^j A^k B^l + \hat{D}_3 f_{ijk} A^i A^j C^k \\ & + \hat{D}_4 f_{ij} A^i E^j + \hat{D}_5 f_{ij} B^i C^j + \hat{D}_6 f_{ijk} A^i B^j B^k + \hat{D}_7 f_{ij} A^i F^j \\ & + \hat{D}_8 f_i I^i + \hat{D}_9 f_i M^i + \hat{D}_{10} f_i P^i + \hat{D}_{11} f_i Q^i + \hat{D}_{12} f_{ij} A^i H^j \\ & + \hat{D}_{13} f_{ij} B^i D^j + \hat{D}_{14} f_{ijk} A^i A^j D^k + \hat{D}_{15} f_{ij} A^i C^j + \hat{D}_{16} f_i K^i \\ & + \hat{D}_{17} f_i N^i + \hat{D}_{18} f_i R^i + \hat{D}_{19} f_i L^i + \hat{D}_{20} f_i J^i, \end{aligned}$$

where

$$\begin{aligned} \hat{D}_i = \tilde{D}_i - \frac{1}{6} \quad (i = 1, 8, 9, 10, 11), \quad \hat{D}_i = \tilde{D}_i - \frac{2}{3} \quad (i = 16, 19), \\ \hat{D}_i = \tilde{D}_i - \frac{1}{2} \quad (i = 17, 18), \quad \hat{D}_i = \tilde{D}_i - \frac{5}{6} \quad (i = 4, 12, 15), \\ \hat{D}_i = \tilde{D}_i - \frac{5}{3} \quad (i = 2, 3, 5, 13, 14), \quad \hat{D}_7 = \tilde{D}_7 - \frac{5}{2}, \\ \hat{D}_{20} = \tilde{D}_{20} - 1, \quad \hat{D}_6 = \tilde{D}_6 - \frac{25}{6}. \end{aligned}$$

We set the error constant C as follows

$$5!C = \sum_{i=1}^{20} |\hat{D}_i|.$$

We have looked for the value r_1 numerically which minimized C , being restricted in the range $-5 \leq r_1 \leq 5$.

The minimum bound on C is achieved if we set $r_1 = -0.4, -0.5$.

In the case $r_1 = -0.5$ the formula (5.2) becomes

$$\begin{aligned} (5.5) \quad K_2 = & F(Y_{n-1} + 1.125hK_1 + 0.375hK_0), \\ K_3 = & F\left(\frac{1}{18}\left(77.948325Y_n - 59.948325Y_{n-1} - \frac{1}{108}\left(307.607625K_1 \right. \right. \right. \\ & \left. \left. \left. + 135.547425K_0 - 186.0651K_2\right)\right)\right), \\ W_0 = & \frac{-25.65}{18006.3}, \quad W_1 = \frac{3316.95}{18006.3}, \quad W_2 = \frac{11115}{18006.3}, \quad W_3 = \frac{3600}{18006.3}, \end{aligned}$$

and the bound for C is

$$C = 0.09.$$

We can prove the stability of the formula (5.2) in the same way as in the proof in Section 3. The estimate formula of local truncation error is given

by (4.5). We compare this method with other methods of order 4 and 5, and present some numerical results in Table IV.

§6. Computational Results

In Tables I, II, III and IV, we present numerical results for the following initial value problems:

$$\text{I: } y' = \frac{y}{x} + \frac{x}{x+1}, \quad y(1) = \log(2), \quad y(x) = x \log(x+1),$$

$$\text{II: } y' = -y - xy^2, \quad y(0) = 1, \quad y(x) = \frac{1}{2e^x - 1 - x},$$

$$\text{III: } y' = -2xy^2, \quad y(0) = 1, \quad y(x) = \frac{1}{1+x^2},$$

$$\text{IV: } y' = \sin(x) - y, \quad y(0) = \frac{1}{2}, \quad y(x) = \frac{1}{2}(\sin(x) - \cos(x)) + e^{-x},$$

$$\text{V: } \begin{cases} y' = -y + z + e^{-x} + e^x, & y(0) = \frac{32}{9}, & y(x) = \frac{5}{9}e^x + e^{-x} + (2+x)e^{-2x} \\ z' = -y - 3z + e^{-x} - e^x, & z(0) = -\frac{17}{9}, & z(x) = \frac{1}{9}e^x - e^{-x} - (1+x)e^{-2x}, \end{cases}$$

$$\text{VI: } \begin{cases} y' = -z, & y(0) = 2, & y(x) = e^x + e^{-3x} \\ z' = -3y - 2z, & z(0) = 2, & z(x) = 3e^{-3x} - e^x, \end{cases}$$

$$\text{VII: } \begin{cases} y' = \frac{1}{z}, & y(0) = 1, & y(x) = e^x \\ z' = -\frac{1}{y}, & z(0) = 1, & z(x) = e^{-x}. \end{cases}$$

Computation are done in double precision arithmetic on the FACOM M-190 of Kyushu University. In Table I, the values y_1 necessary for the evaluation using the formulas (2.8) is computed by the Runge-Kutta method of order 4, and in Tables II, III, IV, the value y_1 necessary for the evaluations using the formulas (2.6), (4.3) are computed by Nyström's method of order 5.

Table I.

Error for the solution to Problems I, II, III and IV. Comparison of errors between the formula (2.8) and other methods of order 3. Mesh size $h=1/2^4$.

x	method	stage	I	II	III	IV
2	A	2	0.2688E-4	-0.1309E -4	-0.7494E-5	-0.3009E-4
	B	2	0.7238E-5	-0.1013E -4	-0.9158E-6	-0.2343E-4
	C	3	-0.9173E-5	-0.6779E -5	-0.3834E-5	-0.9241E-7
	D	2	-0.1995E-6	0.1766E -6	-0.6116E-6	0.3786E-6
5	A		0.8136E-4	-0.3829E -6	-0.1685E-5	0.1831E-4
	B		0.2299E-4	-0.3003E -6	-0.9175E-6	0.1427E-4
	C		-0.2652E-4	-0.1823E -6	-0.3874E-6	-0.1713E-5
	D		-0.5563E-6	0.9685E -8	0.5094E-8	-0.3955E-7
8	A		0.1314E-3	-0.1482E -7	-0.3502E-6	-0.2034E-4
	B		0.3726E-4	-0.1187E -7	-0.1962E-6	-0.1586E-4
	C		-0.4276E-4	-0.7738E -8	-0.7746E-7	0.6312E-6
	D		-0.8928E-6	0.3297E -9	0.1707E-8	0.2011E-7
12	A		0.1976E-3	-0.2611E -9	-0.7987E-7	0.1165E-4
	B		0.5606E-4	-0.2100E -9	-0.4521E-7	0.9064E-5
	C		-0.6425E-4	-0.1388E -9	-0.1640E-7	-0.4381E-5
	D		-0.1339E-5	-0.5640E -11	0.4104E-9	-0.2844E-6

Table II.

Error for the solutions to the Problems I, II, III and IV. Comparison of errors between the formula (2.4) with $a_3=0.4$ and other methods of order 4 and 5. Mesh size $h=1/2^4$.

x	method	stage	I	II	III	IV
2	A'	3	-0.5106E-6	-0.5759E -6	-0.3519E -6	-0.5017E -6
	B'	3	-0.1338E-6	-0.3895E -6	-0.6998E -7	-0.3421E -6
	C'	4	0.1544E-6	-0.1886E -6	-0.9769E -7	0.2252E -7
	C	6	0.2481E-8	0.4269E -8	0.1290E -8	0.3384E-10
	D'	3	0.2021E-8	0.2593E -8	-0.9944E -8	0.3212E -8
5	A'		-0.1408E-5	-0.1388E -7	-0.4608E -6	0.3146E -6
	B'		-0.3853E-6	-0.9782E -8	-0.1748E -7	0.2176E -6
	C'		0.4184E-6	-0.4308E -8	-0.6387E -8	-0.4555E -7
	C		0.6311E-8	0.8901E-10	0.7234E-10	0.2512E -9
	D'		0.5135E-8	0.1606E -9	-0.7636E-10	-0.2796E -9
8	A'		-0.2258E-5	-0.4998E -8	-0.8384E -8	-0.3490E -6
	B'		-0.6188E-6	-0.3718E -9	-0.3243E -8	-0.2467E -7
	C'		0.6708E-6	-0.1770E -9	-0.1096E -9	0.3237E -7
	C		0.1005E-7	0.3558E-11	0.1206E-10	-0.1412E -9
	D'		0.8181E-7	0.5382E-11	-0.6224E-11	0.4344E -9
12	A'		-0.3388E-5	-0.3710E-11	-0.1762E -8	0.1938E -6
	B'		-0.9287E-6	-0.6545E-11	-0.6856E -9	0.1112E -6
	C'		0.1006E-5	-0.3168E-11	-0.2259E -9	-0.7033E -7
	C		0.1504E-7	0.6338E-11	0.2464E-11	0.4505E -9
	D'		0.1224E-7	0.9176E-12	-0.9405E-11	-0.2256E -8

Remarks.

- (1) Methods A and A' are Byrne's Processes of order 3 and 4 respectively.
- (2) Methods B and B' are Costabile's Processes of order 3 and 4 respectively.
- (3) Methods C and C' are Runge-Kutta Processes of order 3 and 4 respectively.
- (4) Method \tilde{C} is Nyström's Process of order 5.
- (5) Methods D' and D are the Processes of (2.4) with $a_2=0.4$, which is due to (2.6), and (2.8) respectively.

Table III.
Local Truncation Error Estimate of the Method (2.6). Mesh size $h=1/2^4$.

x	1.5 ($x_0=1.5-2h$)		2.0 ($x_0=2.0-2h$)		2.5 ($x_0=2.5-2h$)	
	actual error	formula (4.5)	actual error	formula (4.5)	actual error	formula (4.5)
I	0.1518E-9	-0.1475E-9	0.3925E-10	0.3853E-10	0.1344E-10	0.1326E-10
II	0.1824E-8	0.1938E-8	0.9903E-9	0.1044E-10	0.4261E-9	0.4485E-9
III	-0.8446E-9	-0.8540E-9	0.4487E-9	0.4651E-9	0.2028E-9	0.2092E-9
IV	0.2784E-9	-0.2860E-9	0.3582E-9	0.3682E-9	0.3947E-9	0.4057E-9

Table IV.
Error for the solutions to the Problems V, VI and VII. Comparison of errors between the formula (5.5) and other methods of order 4 and 5. Mesh size $h=1/2^4$.

x		Method	Stage	V	VI	VII
1	E ₁	C'	8	-0.2705E-6	-0.1474E-5	0.1210E-5
		\tilde{C}	12	-0.7407E-8	0.5988E-7	0.6784E-9
		E	6	0.3126E-8	0.3579E-6	0.1307E-8
	E ₂	C'		-0.1263E-5	-0.5725E-5	-0.1613E-8
		\tilde{C}		0.3521E-7	0.1660E-6	0.1985E-8
		E		0.8603E-7	0.9990E-6	0.1148E-8
2	E ₁	C'		0.3027E-6	0.1604E-5	0.6529E-5
		\tilde{C}		-0.2601E-7	0.2417E-7	-0.3802E-7
		E		0.2600E-7	0.1465E-6	-0.1889E-7
	E ₂	C'		-0.3100E-5	-0.2321E-5	-0.1178E-6
		\tilde{C}		0.7239E-7	-0.1684E-8	0.2224E-8
		E		0.2999E-7	-0.7751E-8	0.1303E-8
4	E ₁	C'		0.4921E-5	0.2636E-4	0.9505E-4
		\tilde{C}		-0.2338E-6	0.2742E-6	-0.1794E-5
		E		0.1949E-7	0.1675E-5	-0.1039E-5
	E ₂	C'		-0.2442E-4	-0.2636E-4	-0.3140E-7
		\tilde{C}		0.5518E-6	-0.2741E-6	0.1015E-8
		E		0.2375E-6	-0.1674E-5	0.6052E-9
6	E ₁	C'		0.3666E-4	0.2921E-3	0.1037E-2
		\tilde{C}		-0.1733E-3	0.3039E-5	-0.3356E-4
		E		0.1227E-6	0.1865E-4	-0.1992E-4
	E ₂	C'		-0.1807E-3	-0.2921E-3	-0.6278E-8
		\tilde{C}		0.4082E-5	-0.3039E-5	0.2901E-9
		E		0.1770E-5	-0.1865E-4	0.1763E-9

Remarks.

- (1) Method E is the Process using (5.5).
- (2) $E_1 = y(x_n) - y_n$, $E_2 = -z(x_n) - z_n$.

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