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On pseudo-Runge-Kutta methods of the third kind

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1. Introduction

Consider the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0, \tag{1.1}$$

where the function $f(x, y)$ is assumed to be sufficiently smooth. Let $y(x)$ be the solution of this problem,

$$x_n = x_0 + nh \qquad (n = 1, 2,\dots, h > 0), \tag{1.2}$$

and let y_1 be an approximation of $y(x_1)$ obtained by some appropriate method. We are concerned with the case where a pseudo-Runge-Kutta method is used for computing approximations y_j of $y(x_j)$ $(j=2, 3,\dots)$.

Byrne and Lambert [1] introduced pseudo-Runge-Kutta methods of order $r+1$ $(r=2, 3)$ of the form

$$y_{n+1} = y_n + h \textstyle\sum_{i=1}^{r} (p_i k_{i,n} + q_i k_{i,n-1}) \qquad (n = 1, 2,\dots), \tag{1.3}$$

where

$$k_{i,m} = f(x_m + a_i h,\ y_m + h \textstyle\sum_{j=1}^{i-1} b_{ij} k_{j,m}) \qquad (i = 1, 2,\dots, r;\ m = 0, 1,\dots),$$
$$a_1 = 0,\ a_i = \textstyle\sum_{j=1}^{i-1} b_{ij} \qquad (i = 2, 3,\dots, r),$$

and p_i, q_i $(i=1, 2,\dots, r)$ and b_{ij} $(i=2, 3,\dots, r; j=1, 2,\dots, i-1)$ are constants. Gruttke [3] has shown that such a method exists also for $r=4$.

Costabile [2] considered pseudo-Runge-Kutta methods of the second kind of the form

$$y_{n+1} = y_n + h \textstyle\sum_{i=0}^{r} p_i k_i \qquad (n = 1, 2,\dots), \tag{1.4}$$

where

$$k_0 = f(x_{n-1}, y_{n-1}), \quad k_1 = f(x_n, y_n),$$
$$k_i = f(x_n + a_i h,\ y_n + h \textstyle\sum_{j=0}^{i-1} b_{ij} k_j), \quad a_i = \textstyle\sum_{j=0}^{i-1} b_{ij} \qquad (i = 2, 3,\dots, r),$$

and p_i $(i=0, 1,\dots, r)$ and b_{ij} $(i=2, 3,\dots, r; j=0, 1,\dots, i-1)$ are constants. Nakashima [4] proposed those of the third kind which are of the form (1.4) with

$$k_i = f(x_n + a_i h,\ y_n + h \textstyle\sum_{j=0}^{i-1} b_{ij} k_j + c_i(y_n - y_{n-1})),$$
$$a_i = \textstyle\sum_{j=0}^{i-1} b_{ij} + c_i \qquad (i = 2, 3,\dots, r),$$

c_i and b_{ij} $(i=2, 3,\dots, r;\ j=0, 1,\dots, i-1)$ being constants. It is known that a method of each kind of order $r+1$ exists for $r=2, 3$.

The object of this paper is to show that for $r=2, 3$ there exists a pseudo-Runge-Kutta method of the third kind of order $r+2$ which embeds a two-step method of order $r+1$, and to show that for $r=4$ we can construct a pseudo-Runge-Kutta method of the third kind of order $r+2$ and also a two-step method of order $r+1$ by incorporating the first value of f in the next step of integration.

2. Preliminaries

Let

(2.1) $$x_n = x_0 + nh \qquad (n = 1, 2,\dots, h > 0),$$

(2.2) $$y_{n+1} = y_n + h\Phi(x_n, y_n, y_{n-1};\ h) \qquad (n = 1, 2,\dots),$$

(2.3) $$\Phi(x_n, y_n, y_{n-1};\ h) = \textstyle\sum_{i=0}^{r} p_i k_i \qquad (r = 2, 3, 4),$$

(2.4) $$t(x_n, y_n, y_{n-1};\ h) = \textstyle\sum_{i=0}^{r+1} q_i k_i + s(y_n - y_{n-1}),$$

where h is a stepsize,

$$k_0 = f(x_{n-1}, y_{n-1}), \quad k_1 = f(x_n, y_n),$$
$$k_i = f(x_n + a_i h,\ y_n + h \textstyle\sum_{j=0}^{i-1} b_{ij} k_j + c_i(y_n - y_{n-1})) \quad (i = 2, 3,\dots, r),$$
$$k_{r+1} = f(x_{n+1}, y_{n+1}),$$

(2.5) $$\textstyle\sum_{j=0}^{i-1} b_{ij} + c_i = a_i \qquad (i = 2, 3,\dots, r),$$

$q_{r+1}=0$ if $r\neq 4$, and the starting value y_1 is computed by some appropriate method.

Denote by $y(x)$ the solution of (1.1) and let

(2.6) $$T(x;\ h) = y(x) + h\Phi(x, y(x), y(x-h);\ h) - y(x+h),$$

(2.7) $$t(x;\ h) = t(x, y(x), y(x-h);\ h),$$

(2.8) $$t_n = t(x_n, y_n, y_{n-1};\ h),$$

(2.9) $$e_i = -2b_{i0} - c_i + 2\textstyle\sum_{j=2}^{i-1} a_j b_{ij} \qquad (i = 2, 3, 4),$$
$$g_i = 3b_{i0} + c_i + 3\textstyle\sum_{j=2}^{i-1} a_j^2 b_{ij},$$
$$l_i = -4b_{i0} - c_i + 4\textstyle\sum_{j=2}^{i-1} a_j^3 b_{ij},$$
$$m_i = 5b_{i0} + c_i + 5\textstyle\sum_{j=2}^{i-1} a_j^4 b_{ij},$$

$$u_{ij} = (e_j - a_j^2)b_{ij}, \quad v_{ij} = (g_j - a_j^3)b_{ij}, \quad w_{ij} = (l_j - a_j^4)b_{ij}$$
$$(i = 3, 4; j = 2, 3, \ldots, i-1).$$

Let D be the differential operator defined by

$$D = \frac{\partial}{\partial x} + k\frac{\partial}{\partial y}, \quad k = f(x_n, y(x_n)) \tag{2.10}$$

and put

(2.11) $D^j f(x_n, y(x_n)) = T^j$, $D^j f_y(x_n, y(x_n)) = S^j$, $D^j f_{yy}(x_n, y(x_n)) = R^j$ $(j = 1, 2, \ldots)$, $(Df)^2(x_n, y(x_n)) = P$, $(Df_y)^2(x_n, y(x_n)) = Q$, $(D^2f)^2(x_n, y(x_n)) = U$, $f_y(x_n, y(x_n)) = f_y$, $f_{yy}(x_n, y(x_n)) = f_{yy}$, $f_{yyy}(x_n, y(x_n)) = f_{yyy}$.

Then $T(x_n; h)$ can be expanded into power series in h as follows:

(2.12)
$$\begin{aligned} T(x_n; h) = {} & A_1 hk + A_2 h^2 T + (h^3/2)(A_3 T^2 + A_4 f_y T) + (h^4/3!)(B_1 T^3 \\ & + 3B_2 TS + B_3 f_y T^2 + B_4 f_y^2 T) + (h^5/4!)(C_1 T^4 + 6C_2 TS^2 + 4C_3 T^2 S \\ & + 3C_4 f_{yy} P + C_5 f_y T^3 + C_6 f_y^2 T^2 + C_7 f_y^3 T + C_8 f_y TS) + (h^6/5!)(D_1 T^5 \\ & + 10D_2 TS^3 + 10D_3 T^2 S^2 + 5D_4 T^3 S + 10D_5 f_{yy} TT^2 + 15D_6 PR + 15D_7 TQ \\ & + D_8 f_y f_{yy} P + D_9 f_y TS^2 + D_{10} f_y T^2 S + D_{11} f_y^2 TS + D_{12} f_y T^4 + D_{13} f_y^2 T^3 \\ & + D_{14} f_y^3 T^2 + D_{15} f_y^4 T) + (h^7/6!)(E_1 T^6 + 15E_2 TS^4 + 20E_3 T^2 S^3 + \\ & 15E_4 T^3 S^2 + 6E_5 T^4 S + 45E_6 PR^2 + 15E_7 f_{yyy} TP + 60E_8 TT^2 R + \\ & 10E_9 f_{yy} U + 15E_{10} f_{yy} TT^3 + 24E_{11} T^2 Q + E_{12} TSS^2 + E_{13} f_{yy} PS + \\ & E_{14} f_y f_{yy} TT^2 + E_{15} f_y^2 f_{yy} P + E_{16} f_y TQ + E_{17} f_y PR + E_{18} f_y TS^3 + \\ & E_{19} f_y T^2 S^2 + E_{20} f_y T^3 S + E_{21} f_y^2 TS^2 + E_{22} f_y^2 T^2 S + E_{23} f_y^3 TS + \\ & E_{24} f_y T^5 + E_{25} f_y^2 T^4 + E_{26} f_y^3 T^3 + E_{27} f_y^4 T^2 + E_{28} f_y^5 T) + O(h^8), \end{aligned}$$

where

(2.13)
$$\begin{aligned} & A_1 = \textstyle\sum_{j=0}^r p_j - 1, \quad A_2 = -p_0 + \Sigma a_i p_i - 1/2, \\ & A_3 = p_0 + \Sigma a_i^2 p_i - 1/3, \quad A_4 = p_0 + \Sigma e_i p_i - 1/3, \\ & B_1 = -p_0 + \Sigma a_i^3 p_i - 1/4, \quad B_2 = -p_0 + \Sigma a_i e_i p_i - 1/4, \\ & B_3 = -p_o + \Sigma g_i p_i - 1/4, \quad B_4 = B_3 + 3\textstyle\sum_{j=3}^r \sum_{k=2}^{j-1} u_{jk} p_j, \\ & C_1 = p_0 + \Sigma a_i^4 p_i - 1/5, \quad C_2 = p_0 + \Sigma a_i^2 e_i p_i - 1/5, \quad C_3 = p_0 + \Sigma a_i g_i p_i - 1/5, \\ & C_4 = p_0 + \Sigma e_i^2 p_i - 1/5, \; C_5 = p_0 + \Sigma l_i p_i - 1/5, \; C_6 = C_5 + 4\textstyle\sum_{j=3}^r \sum_{k=2}^{j-1} v_{jk} p_j, \\ & C_7 = C_6 + 12u_{32} b_{43} p_4, \quad C_8 = 4C_3 + 3C_5 + 12\textstyle\sum_{j=3}^r \sum_{k=2}^{j-1} (a_j + a_k) u_{jk} p_j, \end{aligned}$$

$$D_1 = -p_0+\Sigma a_i^5 p_i-1/6, \quad D_2 = -p_0+\Sigma a_i^3 e_i p_i-1/6,$$
$$D_3 = -p_0+\Sigma a_i^2 g_i p_i-1/6, \quad D_4 = -p_0+\Sigma a_i l_i p_i-1/6,$$
$$D_5 = -p_0+\Sigma e_i g_i p_i-1/6, \quad D_6 = -p_0+\Sigma a_i e_i^2 p_i-1/6,$$
$$D_7 = D_4+4 \textstyle\sum_{j=3}^r \sum_{k=2}^{j-1} a_j a_k u_{jk} p_j,$$
$$D_8 = 10D_5+3D_{12}+15 \textstyle\sum_{j=3}^r \sum_{k=2}^{j-1} (e_k+a_k^2+2e_j)u_{jk}p_j,$$
$$D_9 = 10D_3+6D_{12}+30 \textstyle\sum_{j=3}^r \sum_{k=2}^{j-1} (a_j^2+a_k^2)u_{jk}p_j,$$
$$D_{10} = 5D_4+4D_{12}+20 \textstyle\sum_{j=3}^r \sum_{k=2}^{j-1} (a_j+a_k)v_{jk}p_j,$$
$$D_{11} = D_{10}+3D_{14}+60(a_3+a_4)u_{32}b_{43}p_4, \quad D_{12} = -p_0+\Sigma m_i p_i-1/6,$$
$$D_{13} = D_{12}+5 \textstyle\sum_{j=3}^r \sum_{k=2}^{j-1} w_{jk}p_j, \quad D_{14} = D_{15} = D_{13}+20v_{32}b_{43}p_4$$

and i ranges from 2 to r. Also $t(x_n; h)$ can be expanded as follows:

$$t(x_n; h) = A_1^*hk + A_2^*h^2T + (h^3/2)(A_3^*T^2+A_4^*f_yT) + (h^4/3!)(B_1^*T^3 + 3B_2^*TS+B_3^*f_yT^2+B_4^*f_y^2T) + \cdots, \tag{2.14}$$

where

$$A_1^* = \textstyle\sum_{j=0}^{r+1} q_j + s, \quad A_2^* = -q_0 + \Sigma a_i q_i + q_{r+1} - s/2, \tag{2.15}$$
$$A_3^* = q_0 + \Sigma a_i^2 q_i + q_{r+1} + s/3, \quad A_4^* = q_0 + \Sigma e_i q_i + q_{r+1} + s/3,$$
$$B_1^* = -q_0 + \Sigma a_i^3 q_i + q_{r+1} - s/4, \quad B_2^* = -q_0 + \Sigma a_i e_i q_i + q_{r+1} - s/4,$$
$$B_3^* = -q_0 + \Sigma g_i q_i + q_{r+1} - s/4, \quad B_4^* = B_3^* + 3 \textstyle\sum_{j=3}^r \sum_{k=2}^{j-1} u_{jk} q_j$$

and so on.

Let

$$d_{ij} = a_j(a_j+1)b_{ij} \qquad (i = 3, 4;\ 2 \leqq j \leqq i-1). \tag{2.16}$$

Then from (2.9) it follows that

$$l_i = -e_i - 2g_i + 2 \textstyle\sum_{j=2}^{i-1} (2a_j+1)d_{ij} \qquad (i = 2, 3, 4),$$
$$m_i = 2e_i + 3g_i + \textstyle\sum_{j=2}^{i-1} (5a_j^2 - 5a_j - 4)d_{ij},$$
$$b_{i0} = e_i + g_i - \textstyle\sum_{j=2}^{i-1} a_j(3a_j+2)b_{ij}, \tag{2.17}$$
$$c_i = -3e_i - 2g_i + 6 \textstyle\sum_{j=2}^{i-1} d_{ij}. \tag{2.18}$$

3. Construction of the methods

We shall show the following

THEOREM. *For* $r=2, 3, 4$ *there exist formulas* (2.2) *and* (2.4) *such that* $T(x_n; h)=O(h^{r+3})$ *and* $t(x_n; h)=O(h^{r+2})$ *respectively.*

3.1. Case $r=2$

The choice $A_i=B_i=0$ $(i=1, 2, 3, 4)$ yields

(3.1) $a_2 = 7/10, \quad b_{20} = 833/1000, \quad b_{21} = 2023/1000, \quad c_2 = -539/250,$

(3.2) $y_{n+1} = y_n + h(-7k_0 + 221k_1 + 500k_2)/714,$

(3.3) $5C_i = -5/24 \ (i = 1, 2, 3, 4), \quad 5C_j = -31/6 \ (j = 5, 6, 7), \quad 5C_8 = -49/3.$

This method has been obtained by Nakashima.

Choosing $A_i^*=0$ $(i=1, 2, 3, 4)$ and $s=1/2$, we have

(3.4) $t_n = h(-287k_0 - 527k_1 + 100k_2)/1428 + (y_n - y_{n-1})/2,$

(3.5) $4B_i^* = 2/5, \quad 5C_i^* = -101/240 \ (i = 1, 2, 3, 4),$

$5C_j^* = -11/12 \ (j = 5, 6, 7), \quad 5C_8^* = -133/30.$

The method (3.2) is of order 4 and the method $z_{n+1}=y_{n+1}+t_n$ is of order 3, so that the difference t_n of the two methods is available for stepsize control.

3.2. Case $r=3$

The conditions $A_i=B_i=0$ $(i=1, 2, 3, 4)$ and $C_j=0$ $(j=1, 2,\dots, 8)$ yield

(3.6) $e_i = a_i^2, \quad g_i = a_i^3 \ (i = 2, 3), \quad 27 - 35(a_2 + a_3) + 50a_2a_3 = 0,$

$\sum_{j=0}^{3} p_i=1, \quad -p_0+a_2p_2+a_3p_3=1/2, \quad 12a_2(a_2+1)(a_2-a_3)p_2=7-10a_3,$

$12a_3(a_3+1)(a_3-a_2)p_3 = 7 - 10a_2, \quad 60(2a_2+1)d_{32}p_3 = 31,$

(3.7) $600D_i=25(a_2+a_3)-31 \ (i=1, 2, 3, 5, 6), \quad 60D_j=62a_3-49 \ (j=4, 7),$

$60D_{12} = (155a_2^2 - 5a_2 - 49)/(2a_2+1),$

$60D_k = -(160a_2+49)/(2a_2+1) \ (k = 13, 14, 15) \quad D_8 = 10D_1 + 3D_{12},$

$D_9 = 10D_1 + 6D_{12}, \quad D_{10} = 5D_4 + 4D_{12}, \quad D_{11} = D_{10} + 3D_{13}.$

The conditions $A_i^*=B_i^*=0$ $(i=1, 2, 3, 4)$ lead to

(3.8) $\sum_{i=0}^{3} q_i + s = 0, \quad -q_0 + a_2q_2 + a_3q_3 = s/2,$

$12a_2(a_2+1)(a_2-a_3)q_2 + (2a_3+1)s = 0,$

$12a_3(a_3+1)(a_3-a_2)q_3 + (2a_2+1)s = 0,$

(3.9) $5C_i^* = 2(5a_2^2 - a_2 - 2)s/(7 - 10a_2) \ (i = 1, 2, 3, 4),$

$5C_j^* = -4(3a_2+1)s/(7-10a_2) \ (j = 5, 6, 7), \quad C_8^* = 3C_1^* + 4C_5^*.$

For $a_2=1/5$ and $s=-1/2$ we have

(3.10) $a_2 = 1/5, \quad b_{20} = 6/125, \quad b_{21} = 36/125, \quad c_2 = -17/125, \quad a_3 = 4/5,$

$b_{30} = -2214/4375, \; b_{31} = -15444/4375, \; b_{32} = 558/175, \; c_3 = 7208/4375,$

(3.11) $y_{n+1} = y_n + h(2k_0 - 81k_1 + 750k_2 + 625k_3)/1296,$

(3.12) $t_n = h(398k_0 + 2673k_1 - 1950k_2 + 175k_3)/2592 - (y_n - y_{n-1})/2,$

(3.13) $6D_i = -3/50 \; (i = 1, 2, 3, 5, 6), \quad 6D_j = 3/50 \; (j = 4, 7),$

$6D_8 = -699/70, \quad 6D_9 = -678/35, \quad 6D_{10} = -2157/70,$

$6D_{11} = -1686/35, \quad 6D_{12} = -219/70, \quad 6D_k = -81/14 \; (k = 13, 14, 15),$

(3.14) $5C_i^* = 2/5 \; (i = 1, 2, 3, 4), \quad 5C_j^* = 16/25 \; (j = 5, 6, 7), \quad 5C_8^* = 94/25.$

3.3. Case $r=4$

If we impose the condition $a_2(a_2+1) \neq 0$ and choose

$A_i = B_i = 0 \; (i = 1, 2, 3, 4), \quad C_j = 0 \; (j = 1, 2, \dots, 8), \quad D_k = 0 \; (k = 1, 2, \dots, 15),$
then we have

(3.15) $b_{32}b_{43}(a_4 - a_3)p_4 \neq 0, \quad e_i = a_i^2, \quad g_i = a_i^3 \; (i = 2, 3, 4), \quad a_4 = 1,$

$5 - 8(a_2 + a_3) + 15a_2a_3 = 0, \quad \sum_{j=0}^4 p_j = 1, \quad -p_0 + \sum_{i=2}^4 p_i = 1/2,$

$60a_2(a_2+1)(a_2-1)(a_2-a_3)p_2 = 15a_3 - 8,$

$60a_3(a_3+1)(a_3-1)(a_3-a_2)p_3 = 15a_2 - 8,$

$120(1-a_2)(1-a_3)p_4 = 27 - 35(a_2+a_3) + 50a_2a_3,$

$120(1-a_3)(2a_2+1)d_{32}p_3 = 13,$

$60(3+5a_2+5a_3+10a_2a_3)(a_3-a_2)d_{43}p_4 = 49 + 5a_2 - 155a_2^2,$

$120(1-a_3)[(2a_2+1)d_{42} + (2a_3+1)d_{43}]p_4 = 49 - 62a_3.$

The choice $A_i^* = B_i^* = 0 \; (i=1, 2, 3, 4)$ and $C_j^* = 0 \; (j=1, 2, \dots, 8)$ yields

(3.16) $\sum_{j=0}^5 q_j + s = 0, \quad -q_0 + \sum_{i=2}^4 a_iq_i + q_5 = s/2,$

$60a_2(a_2+1)(a_2-1)(a_2-a_3)q_2 = (15a_3+8)s,$

$60a_3(a_3+1)(a_3-1)(a_3-a_2)q_3 = (15a_2+8)s,$

$120(1-a_2)(1-a_3)(q_4+q_5) = (3+5a_2+5a_3+10a_2a_3)s,$

$(2a_2+1)d_{32}q_3 + [(2a_2+1)d_{42} + (2a_3+1)d_{43}]q_4 + 2q_5 + s/60 = 0,$

(3.17) $D_i^* = 4(a_2+a_3)s/15 \; (i = 1, 2, 3, \dots, 6),$

$D_j^* = 2(a_3-1)(2a_2+1)d_{32}q_3 - s/20 \; (j = 4, 7),$

$D_{12}^* = a_2(5a_2+3)d_{32}q_3 + [a_2(5a_2+3)d_{42} + a_3(5a_3+3)d_{43}]q_4 + 4q_5 - s/60,$

$$D_k^* = -2a_2d_{32}q_3 - 2[a_2d_{42} + a_3d_{43} - 5(2a_2+1)d_{32}b_{43}]q_4 + 4q_5 - s/60$$

$$(k = 13, 14, 15),\quad D_8^* = 10D_1^* + 3D_{12}^*,\quad D_9^* = 10D_1^* + 6D_{12}^*,$$

$$D_{10}^* = 5D_4^* + 4D_{12}^*,\quad D_{11}^* = D_{10}^* + 3D_{13}^*.$$

For $a_2 = 1/6$ and $s = 1/20$ we have

(3.18) $a_2 = 1/6,\ b_{20} = 7/216,\ b_{21} = 49/216,\ c_2 = -5/54,\ a_3 = 2/3,$
$b_{30} = -2615/8316,\ b_{31} = -3065/1188,\ b_{32} = 195/77,\ c_3 = 611/594,$
$a_4 = 1,\ b_{40} = 2399/1708,\ b_{41} = 2821/244,\ b_{42} = -3825/427,$
$b_{43} = 99/61,\ c_4 = -565/122,$

(3.19) $y_{n+1} = y_n + h(k_0 - 35k_1 + 1728k_2 + 2079k_3 + 427k_4)/4200,$

(3.20) $t_n = h(-1111k_0 - 15715k_1 + 15552k_2 - 3969k_3 + 1043k_4)/84000$
$+ 13h(k_4 - k_5)/220 + (y_n - y_{n-1})/20,$

(3.21) $7E_i = 19/1080\ (i=1, 2, 3, 6, 7, 8, 9),\ 7E_j = -1/36\ (j = 4, 10),$
$7E_k = 3571/5760\ (k = 5, 11),\ 7E_{12} = 3371/160,\ 7E_{13} = 3171/320,$
$7E_{14} = 13487/108,\ 7E_{15} = 261523/1728,\ 7E_{16} = 27289/120,$
$7E_{17} = 6785/36,\ 7E_{18} = 6766/54,\ 7E_{19} = 75599/540,$
$7E_{20} = 17009/720,\ 7E_{21} = 148093/1440,\ 7E_{22} = 38301/360,$
$7E_{23} = 163759/1440,\ 7E_{24} = 2249/180,\ 7E_{25} = 1705/192,$
$7E_m = 267/48\ (m = 26, 27, 28),$

(3.22) $6D_i^* = 1/15\ (i=1, 2, 3, 5, 6),\ 6D_j^* = 6/55\ (j=4, 7),\ 6D_8^* = -2173/2640,$
$6D_9^* = -3053/1320,\ 6D_{10}^* = -317/220,\ 6D_{11}^* = -493/110,$
$6D_{12}^* = -437/880,\ 6D_k^* = -223/220\ (k = 13, 14, 15).$

If y_{n+1} is accepted as an approximation to $y(x_{n+1})$, then k_5 can be used as k_1 in the next step of integration.

Added in proof: After the submission of this work, we learned that M. Nakashima has obtained independently an optimal pseudo-Runge-Kutta method of the third kind of order 5 for $r=3$.

References

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