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FAMILIES OF THREE-STAGE THIRD ORDER RUNGE-KUTTA-NYSTRÖM METHODS FOR $y'' = f(x, y, y')$

M. M. CHAWLA[1] AND S. R. SHARMA[2]

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Abstract

In this paper all three-stage third order (explicit) Runge-Kutta-Nyström (R-K-N) methods for $y'' = f(x, y, y')$ are presented. While determining particular methods we require that when these methods are applied to the test equation: $y'' - (\alpha + \beta)y' + \alpha\beta y = 0$, the measure of the relative error F, introduced by Rutishauser [4], should not deteriorate in the case of equal eigenvalues ($\beta \to \alpha$). Further, we require that when these methods are applied to special differential equations $y'' = f(x, y)$ they should possess either of the two properties: (P1) a method remains of order three but is two-stage, (P2) a method remains three-stage but attains order four. We present new R-K-N methods which are stabilized in the sense of Ruthishauser [4] and which possess the property (P1). (There does not exist any three-stage third order R-K-N method which is stabilized and which possesses the property (P2).)

1. Introduction

For the second order initial value problem:

$$y'' = f(x, y, y'), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \tag{1}$$

consider a general three-stage (explicit) R-K-N method defined by

$$y_{k+1} = y_k + hy'_k + h^2(a_1K_1 + a_2K_2 + a_3K_3) + T_k(h), \tag{2a}$$

$$y'_{k+1} = y'_k + h(b_1K_1 + b_2K_2 + b_3K_3) + T'_k(h), \tag{2b}$$

[1]Department of Mathematics, Indian Institute of Technology, Hauz Khas, New Delhi-110016, India.
[2]Department of Mathematics, Deshbandhu College, Kalkaji, New Delhi-110019, India.
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where

$$K_1 = f(x_k + \alpha_1 h, y_k + \alpha_1 h y_k', y_k'),$$

$$K_2 = f\big(x_k + \alpha_2 h, y_k + \alpha_2 h y_k' + h^2 \beta_{21} K_1, y_k' + h\gamma_{21} K_1\big),$$

$$K_3 = f\big(x_k + \alpha_3 h, y_k + \alpha_3 h y_k' + h^2(\beta_{31} K_1 + \beta_{32} K_2), y_k' + h(\gamma_{31} K_1 + \gamma_{32} K_2)\big),$$

and $T_k(h)$, $T_k'(h) = O(h^4)$. In contrast to the usual Taylor series expansion method using differential operators, Hairer and Wanner [2] have given an interesting application of certain tree structures for obtaining the necessary equations of conditions governing the parameters for R-K-N methods of various orders. They also indicate how numerical methods could be obtained from the equations of conditions; however, no complete solutions of these equations of conditions have been given so far.

In the present paper we obtain all possible families of three-stage third order (explicit) R-K-N methods for the initial value problem (1). For a general R-K-N method defined by (2); there result twelve equations of conditions necessary for order three involving the fifteen parameters: a_i, b_i, α_i, $i = 1, 2, 3$; $\beta_{21}, \beta_{31}, \beta_{32}, \gamma_{21}, \gamma_{31}, \gamma_{32}$. In Section 2 we first establish two propositions concerning these equations of conditions. With the help of these propositions we obtain an equivalent system of twelve equations which essentially characterizes all possible third order R-K-N methods. For $\alpha_1 = 0$, this equivalent system of necessary conditions reduces to nine equations in fourteen parameters and we obtain a five-parameter family of methods. For $\alpha_1 \neq 0$, the system necessarily implies $a_1 = b_1 = 0$, and we obtain a three-parameter family of methods. In Section 3 we discuss stability of the families of methods obtained in Section 2. Rutishauser [4] introduced the measure of the relative error F and suggested the asymptotic ($x \to \infty$) behaviour of F (F_∞) as a criterion for the performance of a numerical method for integration over a large interval. Following Rutishauser [4], while determining particular methods from the families of methods obtained in Section 2, we require that when these methods are applied to the test equation: $y'' - (\alpha + \beta)y' + \alpha\beta y = 0$, the asymptotic relative error F_∞ should not deteriorate when $\beta \to \alpha$ (the case of equal eigenvalues). In Section 4 we characterize those third order R-K-N methods which when applied to special second order differential equations $y'' = f(x, y)$ possess either of the two properties: (P1) a method remains of order three but is two-stage, (P2) a method remains three-stage but attains order four. In Section 5 we present new R-K-N methods which are stabilized in the sense of Rutishauser [4] and which possess the property (P1). (There does not exist any three-stage third order R-K-N method which is stabilized and which possesses the property (P2)).

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2. Order conditions and their solutions

In order that $T_k(h), T_k'(h) = O(h^4)$ for a method described by (2), there results (see Hairer and Wanner [2], Table 1) the following system of twelve equations necessary for order three

$$a_1 + a_2 + a_3 = \tfrac{1}{2}, \tag{3a}$$
$$a_1\alpha_1 + a_2\alpha_2 + a_3\alpha_3 = \tfrac{1}{6}, \tag{3b}$$
$$a_2\gamma_{21} + a_3(\gamma_{31} + \gamma_{32}) = \tfrac{1}{6}, \tag{4}$$
$$b_1 + b_2 + b_3 = 1, \tag{5a}$$
$$b_1\alpha_1 + b_2\alpha_2 + b_3\alpha_3 = \tfrac{1}{2}, \tag{5b}$$
$$b_1\alpha_1^2 + b_2\alpha_2^2 + b_3\alpha_3^2 = \tfrac{1}{3}, \tag{5c}$$
$$b_2\gamma_{21} + b_3(\gamma_{31} + \gamma_{32}) = \tfrac{1}{2}, \tag{6a}$$
$$b_2\gamma_{21}^2 + b_3(\gamma_{31} + \gamma_{32})^2 = \tfrac{1}{3}, \tag{6b}$$
$$b_2\alpha_2\gamma_{21} + b_3\alpha_3(\gamma_{31} + \gamma_{32}) = \tfrac{1}{3}, \tag{6c}$$
$$b_2\gamma_{21}\alpha_1 + b_3(\gamma_{31}\alpha_1 + \gamma_{32}\alpha_2) = \tfrac{1}{6}, \tag{7a}$$
$$b_3\gamma_{32}\gamma_{21} = \tfrac{1}{6}, \tag{7b}$$
$$b_2\beta_{21} + b_3(\beta_{31} + \beta_{32}) = \tfrac{1}{6}. \tag{8}$$

From (7b) it follows that

$$b_3 \neq 0, \qquad \gamma_{32} \neq 0, \qquad \gamma_{21} \neq 0. \tag{9}$$

This shows that no third order R-K-N method can be based on two evaluations of f.

We first establish the following results which help in obtaining complete solutions of the system (3)–(8). In the following we set:

$$d_1 = -\alpha_1, \qquad d_2 = \gamma_{21} - \alpha_2, \qquad d_3 = \gamma_{31} + \gamma_{32} - \alpha_3. \tag{10}$$

Proposition 1. *The system* (3)–(8) *necessarily implies that*

$$b_1d_1 = b_2d_2 = b_3d_3 = 0. \tag{11}$$

Proof. Our proof makes use of Lemma 1 in Butcher [1]. Let U, V and W be the matrices described by

$$U = \begin{bmatrix} b_1 & b_2 & b_3 \\ b_1\alpha_1 & b_2\alpha_2 & b_3\alpha_3 \\ b_1d_1 & b_2d_2 & b_3d_3 \end{bmatrix}, \qquad V = \begin{bmatrix} 1 & \alpha_1 & d_1 \\ 1 & \alpha_2 & d_2 \\ 1 & \alpha_3 & d_3 \end{bmatrix},$$

$$W = \begin{bmatrix} 1 & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

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From the order condition $UV = W$. Since W is singular either U or V is singular, and from $\mathbf{u}^T U = \mathbf{0}$ it follows that $\mathbf{u}^T W = \mathbf{0}$ implying that $\mathbf{u}^T$ is a scalar multiple of $(0, 0, 1)$. Thus $\mathbf{u}^T U = \mathbf{0}$ implies (11). Similarly if V is singular then $d_1 = d_2 = d_3 = 0$ implying again (11).

PROPOSITION 2. *The system* (3)–(8) *necessarily implies that*

$$d_2 = d_3 = 0. \tag{12}$$

PROOF. From (7b) and (11) we obtain $d_3 = 0$. For $\alpha_1 = 0$ from (7) we obtain $d_2 = 0$; for $\alpha_1 \neq 0$ from (5) and (11) it follows that $d_2 = 0$.

As a consequence of Proposition 2 from (3b) and (4), (5b) and (6a), (7a) and (7b) it immediately follows that

$$a_1\alpha_1 = b_1\alpha_1 = (b_2\gamma_{21} + b_3\gamma_{31})\alpha_1 = 0. \tag{13}$$

Now from the above results it follows that the system (3)–(8) is equivalent to the following system, S, of twelve equations.

$$S: \quad (3), (5), (7\text{b}), (8), (12), (13).$$

Thus all third order R-K-N methods are essentially characterized by the system S and all possible families of third order R-K-N methods can be obtained from this system.

We next obtain the families of third order R-K-N methods. From the system S (see (13)) it is clear that we need obtain families of methods for the two cases: (i) $\alpha_1 = 0$, (ii) $\alpha_1 \neq 0$.

2.1 Families of third order R-K-N methods for $\alpha_1 = 0$

For the case $\alpha_1 = 0$, equations in (13) are identically satisfied and the system S now reduces to a system of nine equations in fourteen parameters and a five-parameter family of methods can be obtained. With α_2, α_3, a_3, β_{21}, β_{32} chosen as free parameters, the remaining parameters are as given in the following.

$$\begin{aligned}
&\alpha_1 = 0,\\
&a_1 = [3\alpha_2 - 1 + 6a_3(\alpha_3 - \alpha_2)]/(6\alpha_2),\\
&a_2 = (1 - 6a_3\alpha_3)/(6\alpha_2),\\
&b_2 = (3\alpha_3 - 2)/[6\alpha_2(\alpha_3 - \alpha_2)],\\
&b_3 = (3\alpha_2 - 2)/[6\alpha_3(\alpha_2 - \alpha_3)],\\
&b_1 = 1 - b_2 - b_3,\\
&\gamma_{21} = \alpha_2,\\
&\gamma_{32} = [\alpha_3(\alpha_2 - \alpha_3)]/[\alpha_2(3\alpha_2 - 2)],\\
&\gamma_{31} = \alpha_3 - \gamma_{32}.\\
&\beta_{31} = 1/6b_3 - (b_2/b_3)\beta_{21} - \beta_{32}.
\end{aligned} \tag{14}$$

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This solution is valid provided $\alpha_2 \neq 0$, $\alpha_2 \neq \frac{2}{3}$, $\alpha_3 \neq 0$ and $\alpha_2 \neq \alpha_3$. This family of third order R-K-N methods will be denoted by $M_3(\alpha_2, \alpha_3; a_3; \beta_{21}, \beta_{32})$.

Now, from (7b) and (12) it follows that $\alpha_2 \neq 0$. Since $b_3 \neq 0$, from the above expression for b_3 it is easy to see that α_2 cannot be equal to $\frac{2}{3}$ unless either $\alpha_3 = 0$ or $\alpha_2 = \alpha_3$; this possibility will be covered in the cases: (a) $\alpha_3 = 0$, (b) $\alpha_2 = \alpha_3$. For each of these two cases, a four-parameter family of methods are possible as listed below.

(a) Families of methods for $\alpha_1 = 0$ and $\alpha_3 = 0$

With a_3, b_3, β_{21} and β_{32} chosen as the free parameters, the remaining parameters are as given in the following.

$$\begin{aligned} &\alpha_1 = \alpha_3 = 0, \qquad \alpha_2 = \tfrac{2}{3}, \\ &a_1 = \tfrac{1}{4} - a_3, \qquad a_2 = \tfrac{1}{4}, \\ &b_1 = \tfrac{1}{4} - b_3, \qquad b_2 = \tfrac{3}{4}, \\ &\gamma_{21} = \tfrac{2}{3}, \qquad \gamma_{31} = -1/4b_3, \qquad \gamma_{32} = 1/4b_3, \\ &\beta_{31} = 1/6b_3 - (3/4b_3)\beta_{21} - \beta_{32}. \end{aligned} \tag{15}$$

This family of third order R-K-N methods will be denoted by $M_3^{(1)}(a_3, b_3; \beta_{21}, \beta_{32})$.

(b) Families of methods for $\alpha_1 = 0$ and $\alpha_2 = \alpha_3$

With a_3, b_3, β_{21}, β_{32} chosen as the free parameters, the remaining parameters are as given in the following.

$$\begin{aligned} &\alpha_1 = 0, \qquad \alpha_2 = \alpha_3 = \tfrac{2}{3}, \\ &a_1 = \tfrac{1}{4}, \qquad a_2 = \tfrac{1}{4} - a_3, \\ &b_1 = \tfrac{1}{4}, \qquad b_2 = \tfrac{3}{4} - b_3, \\ &\gamma_{21} = \tfrac{2}{3}, \qquad \gamma_{31} = \tfrac{2}{3} - 1/4b_3, \qquad \gamma_{32} = 1/4b_3, \\ &\beta_{31} = 1/6b_3 - (b_2/b_3)\beta_{21} - \beta_{32}. \end{aligned} \tag{16}$$

This family of third order R-K-N methods will be denoted by $M_3^{(2)}(a_3, b_3; \beta_{21}, \beta_{32})$.

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2.2 Families of third order R-K-N methods for $\alpha_1 \neq 0$

In this case from (13) it follows that $a_1 = b_1 = 0$; then, in the system S there remain ten equations in thirteen parameters and a three-parameter family of methods can be obtained. With α_1, β_{21} and β_{32} chosen as the free parameters, the remaining parameters are as given in the following.

$$\begin{aligned} &\alpha_2 = \tfrac{1}{3}, \quad \alpha_3 = 1, \\ &a_1 = 0, \quad a_2 = \tfrac{1}{2}, \quad a_3 = 0, \\ &b_1 = 0, \quad b_2 = \tfrac{3}{4}, \quad b_4 = \tfrac{1}{4}, \\ &\gamma_{21} = \tfrac{1}{3}, \quad \gamma_{31} = -1, \quad \gamma_{32} = 2, \\ &\beta_{31} = \tfrac{2}{3} - 3\beta_{21} - \beta_{32}. \end{aligned} \tag{17}$$

This family of third order R-K-N methods will be denoted by $M_3^*(\alpha_1; \beta_{21}, \beta_{32})$.

3. Stability of the methods

Following Rutishauser [4] we consider the test equation:

$$y'' - (\alpha + \beta) y' + \alpha\beta y = 0. \tag{18}$$

Let $Y_k = [y_k, y_k']^T$; then the exact solution of (18) at $x = x_0 + kh$ can be written as

$$Y_k = e^{khA} y_0, \tag{19}$$

where

$$A = \begin{bmatrix} 0 & 1 \\ -\alpha\beta & \alpha + \beta \end{bmatrix}.$$

Let $\tilde{Y}_k = [\tilde{y}_k, \tilde{y}_k']^T$ denote the numerical approximation for Y_k obtained by a method defined by (2) neglecting $T_k(h)$, $T_k'(h)$. For the numerical integration of the differential equation (8) by a method described by (2) we may write

$$\tilde{Y}_{k+1} = C\tilde{Y}_k, \qquad k = 0, 1, 2, \ldots. \tag{20}$$

Let $C = (c_{ij})_{i,j=1}^2$; then, with the help of the system (3)–(8) we find that for a method defined by (2),

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$$c_{11} = 1 - \alpha\beta h^2/2 - \alpha\beta(\alpha+\beta)h^3/6$$
$$+\alpha\beta\left[\alpha\beta\{a_2\beta_{21} + a_3(\beta_{31}+\beta_{32})\} - (\alpha+\beta)^2 a_3\gamma_{32}\alpha_2\right]h^4$$
$$+\alpha^2\beta^2(\alpha+\beta)a_3(\beta_{32}\gamma_{21}+\gamma_{32}\beta_{21})h^5 - \alpha^3\beta^3 a_3\beta_{32}\beta_{21}h^6,$$
$$c_{12} = h\big[1 + (\alpha+\beta)h/2 + (\alpha^2+\alpha\beta+\beta^2)h^2/6$$
$$-(\alpha+\beta)\{\alpha\beta(a_2\beta_{21} + a_3(\beta_{31}+\beta_{32})$$
$$+a_2\gamma_{21}\alpha_1 + a_3(\gamma_{31}\alpha_1+\gamma_{32}\alpha_2)) - (\alpha+\beta)^2 a_3\gamma_{32}\gamma_{21}\}h^3$$
$$+\alpha\beta\{\alpha\beta(a_2\beta_{21}\alpha_1 + a_3(\beta_{31}\alpha_1+\beta_{32}\alpha_2))$$
$$-(\alpha+\beta)^2 a_3(\beta_{32}\gamma_{21}+\gamma_{32}\beta_{21}+\gamma_{32}\gamma_{21}\alpha_1)\}h^4$$
$$+\alpha^2\beta^2(\alpha+\beta)a_3\{\beta_{32}\beta_{21} + (\gamma_{32}\beta_{21}+\beta_{32}\gamma_{21})\alpha_1\}h^5$$
$$-\alpha^3\beta^3 a_3\beta_{32}\beta_{21}\alpha_1 h^6\big],$$
$$c_{21} = -\alpha\beta h\big[1 + (\alpha+\beta)h/2 + (\alpha^2+\alpha\beta+\beta^2)h^2/6$$
$$-\alpha\beta(\alpha+\beta)b_3(\beta_{32}\gamma_{21}+\gamma_{32}\beta_{21})h^3 + \alpha^2\beta^2 b_3\beta_{32}\beta_{21}h^4\big],$$
$$c_{22} = 1 + (\alpha+\beta)h + (\alpha^2+\alpha\beta+\beta^2)h^2/2 + (\alpha+\beta)(\alpha^2+\beta^2)h^3/6$$
$$+\alpha\beta\{\alpha\beta(b_2\beta_{21}\alpha_1 + b_3(\beta_{31}\alpha_1+\beta_{32}\alpha_2))$$
$$-(\alpha+\beta)^2 b_3(\beta_{32}\gamma_{21}+\gamma_{32}\beta_{21}+\gamma_{32}\gamma_{21}\alpha_1)\}h^4$$
$$+\alpha^2\beta^2(\alpha+\beta)b_3(\beta_{32}\beta_{21}+\beta_{32}\gamma_{21}\alpha_1+\gamma_{32}\beta_{21}\alpha_1)h^5$$
$$-\alpha^3\beta^3 b_3\beta_{32}\beta_{21}\alpha_1 h^6. \tag{21}$$

We discuss stability of the families of numerical methods obtained in Section 2 by applying these methods to the test equation (18) for which the solutions are exponential. Following Rutishauser [4] we introduce the relative-error function defined by

$$F = (\log y(x) - \log \tilde{y}(x))/(x - x_0), \tag{22}$$

(relative-error per unit length of the integration interval).

The asymptotic ($x \to \infty$) behaviour of the error-function F is described by

$$F_\infty \simeq (\alpha h - \log\lambda)/h, \qquad x = kh, \tag{23}$$

where α is an eigenvalue with greatest real part of the matrix A and λ is an eigenvalue with largest absolute value of the matrix C. For the test equation (18), assuming $\alpha > \beta$, the absolutely largest eigenvalue of the matrix C which, for small h, lies in the neighbourhood of $e^{\alpha h}$ is given by

$$\lambda \simeq e^{\alpha h} - \left[D(e^{\alpha h})/D'(e^{\alpha h})\right], \tag{24}$$

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where $D(\lambda) = |C - \lambda I|$, I being the unit matrix. With the help of (24) from (25) we get

$$F_\infty \simeq \frac{g(\alpha, \beta)h^3 + O(h^4)}{(\alpha - \beta) + O(h)}, \tag{25}$$

where

$$\begin{aligned} g(\alpha, \beta) = & -\alpha^3\beta^2\{a_2\beta_{21} + a_3(\beta_{31} + \beta_{32})\} \\ & +\alpha^3\beta(\alpha + \beta)(a_3\gamma_{32}\alpha_2 + b_3\gamma_{32}\beta_{21}) + \alpha^4\beta b_3\beta_{32}\alpha_2 \\ & -\{\alpha^3\beta^2(b_2\beta_{21} + b_3\beta_{31}) \\ & +\alpha^2\beta^2(\alpha + \beta)(a_2\gamma_{21} + a_3\gamma_{31}) - \tfrac{1}{6}\alpha^2\beta(\alpha + \beta)^2\}\alpha_1 \\ & +\alpha^4(\alpha - \beta)/24. \end{aligned}$$

The behaviour of a particular numerical method for integration over a large interval may therefore be adjudged by the measure of the relative-error F_∞. It may be noted that when $\alpha \to \beta$, (25) indicates a possible deterioriation of the approximations provided by a method. This type of deterioration of the relative-error F_∞ for the classical fourth order Runge-Kutta-Nyström method was first pointed out by Rutishauser [4]. Consequently, while looking for "good" methods from the families of methods obtained in Section 2 we essentially require these methods to be stabilized in the sense that when $\alpha \to \beta$ (case of equal eigenvalues) F_∞ does not deteriorate. In order that a method possesses the above stability property we require that $(\alpha - \beta)$ should be a factor of $g(\alpha, \beta)$; hence, we must have

$$\begin{aligned} [a_2\beta_{21} + a_3(\beta_{31} + \beta_{32}) - b_3\beta_{32}\alpha_2 - 2a_3\gamma_{32}\alpha_2 - 2b_3\gamma_{32}\beta_{21} \\ + (b_2\beta_{21} + b_3\beta_{31} + 2a_2\alpha_2 + 2a_3\gamma_{31} - \tfrac{2}{3})\alpha_1] = 0. \end{aligned} \tag{26}$$

"Best" three-stage third order R-K-N methods which are stabilized and which also possess enchanced behaviour when applied to the special differential equations are presented in Section 5.

4. Three-stage third order R-K-N methods as applied to special differential equations $y'' = f(x, y)$

In Section 2 we have given all possible families of three-stage third order R-K-N methods for the general second order initial value problem (1). In this Section we consider finding those three-stage third order R-K-N methods which when applied to special second order differential equations:

$$y'' = f(x, y), \tag{27}$$

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possess either of the following two properties:

(P1): a method remains of order three but is two-stage when applied to (27),

(P2): a method remains three-stage but attains order four when applied to (27).

Methods from the general three-stage third order R-K-N families $M_3(\alpha_2, \alpha_3; a_3; \beta_{21}, \beta_{32})$, $M_3^{(1)}(a_3, b_3; \beta_{21}, \beta_{32})$, $M_3^{(2)}(a_3, b_3; \beta_{21}, \beta_{32})$ and $M_3^*(\alpha_1; \beta_{21}, \beta_{32})$ possessing the property (P1) or (P2) are given, respectively in Sections 4.1 and 4.2.

4.1 Methods possessing property (P1)

A general three-stage R-K-N method given by (2) will reduce to a two-stage method for $y'' = f(x, y)$ provided, at least, one of the following conditions is satisfied:

$$\text{(i) } K_1 = K_2; \qquad \text{(ii) } K_2 = K_3, \qquad \text{(iii) } K_3 = K_1,$$

$$\text{(iv) } a_1 = b_1 = \beta_{21} = \beta_{31} = 0, \qquad \text{(v) } a_2 = b_2 = \beta_{32} = 0.$$

It can now be verified that the following methods/subfamilies of $M_3(\alpha_2, \alpha_3; a_3; \beta_{21}, \beta_{32})$, $M_3^{(1)}(a_3, b_3; \beta_{21}, \beta_{32})$, $M_3^{(2)}(a_3, b_3; \beta_{21}, \beta_{32})$ and $M_3^*(\alpha_1; \beta_{21}, \beta_{32})$ possess the property (P1):

$$M_3(\bar{\alpha}_2, \bar{\alpha}_3; \bar{a}_3; 0, \bar{\beta}_{32}), \qquad M_3(\alpha_2, \tfrac{2}{3}; \tfrac{1}{4}; \beta_{21}, 0), \qquad M_3^{(1)}(a_3, b_3; \tfrac{2}{9}, 0),$$

$$M_3^{(1)}(\tfrac{1}{4}; \tfrac{1}{4}; 0, \tfrac{2}{3}), \qquad M_3^{(2)}(a_3, b_3; \tfrac{2}{9}, 0), \qquad M_3^{(2)}(\tfrac{1}{4}, \tfrac{3}{4}; \beta_{21}, 0),$$

$$M_3^*(\tfrac{1}{3}; 0, \beta_{32}), \qquad M_3^*(1; \tfrac{2}{9}, 0), \qquad M_3^*(\alpha_1; 0, \tfrac{2}{3}),$$

where

$$\bar{\alpha}_3 = \frac{2 - 3\alpha_2}{3(1 - 2\alpha_2)}, \qquad \bar{a}_3 = \frac{(1 - 2\alpha_2)(1 - 3\alpha_2)}{4(1 - 3\alpha_2 + 3\alpha_2^2)},$$

$$\bar{\beta}_{32} = \frac{2(1 - 3\alpha_2 + 3\alpha_2^2)}{9(1 - 2\alpha_2)^2}, \qquad (\alpha_2 \neq \tfrac{1}{2}).$$

In particular we note that both the methods $M_3^{(1)}(\tfrac{1}{4}, \tfrac{1}{4}; \tfrac{2}{9}, 0)$ and $M_3^{(2)}(\tfrac{1}{4}, \tfrac{3}{4}; \tfrac{2}{9}, 0)$ reduce to the classical two-stage third order Nyström method when y' is absent (see Henrici [3]).

4.2 Methods possessing property (P2)

It can be verified that no method of $M_3^{(1)}(a_3, b_3; \beta_{21}, \beta_{32})$, $M_3^{(2)}(a_3, b_3; \beta_{21}, \beta_{32})$ or $M_3^*(\alpha_1; \beta_{21}, \beta_{32})$ has fourth order accuracy when y' is absent.

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It can be shown (we omit details) that each method of the subfamily $M_3(\alpha_2, \alpha_3^*; a_3^*; \beta_{21}^*, :\beta_{32}^*)$ $(= M_4(\alpha_2))$ with

$$\alpha_3^* = \frac{3 - 4\alpha_2}{2(2 - 3\alpha_2)}, \qquad \left(\alpha_2 \neq \tfrac{2}{3}, \tfrac{3}{4}\right), \qquad a_3^* = b_3(1 - \alpha_3^*),$$
$$\beta_{21}^* = \tfrac{1}{2}\alpha_2^2, \qquad \beta_{32}^* = 1/(24 b_3 \alpha_2),$$

possess the property (P2). We note, in particular, that the method $M_3(\frac{1}{2}, 1; 0; \frac{1}{8}, \frac{1}{2}) = M_4(\frac{1}{2})$ reduces to the classical three-stage fourth order Nyström method when y' is absent (see Henrici [3]).

5. "Best" three-stage third order R-K-N methods

In Section 2 we derived all possible three-stage third order R-K-N methods. In Section 3 we considered stability of these methods in the sense of Rutishauser by applying these methods to the test equation (18). In particular we noted that the asymptotic relative error will not deteriorate in case of equal eigenvalues if (26) is satisfied. Thus while selecting particular R-K-N methods we require that for these methods the condition (26) be satisfied. In Section 4 we considered finding those three-stage third order R-K-N methods which when applied to special second order differential equations $y'' = f(x, y)$ possess either the property (P1) or the property (P2).

In this section we present new R-K-N methods which are stabilized in the sense of Rutishauser [4] and which possess either the property (P1) or the property (P2). (In addition we require that $\alpha_1, \alpha_2, \alpha_3 \in [0, 1]$ and $a_i, b_i \geqslant 0$ for $i = 1, 2, 3$.)

First consider determining methods which satisfy (26) and possess the property (P2) when y' is absent. From the discussion in Section 4.2 it can be seen that no method of $M_3(\alpha_2, \alpha_3^*; a_3^*, \beta_{21}^*, \beta_{32}^*)$ exist satisfying (26). Consequently no three-stage third order R-K-N method exists for which the condition (26) is satisfied and which attains order four when y' is absent.

Next, we consider determining those three-stage third order R-K-N methods which satisfy the condition (26) and possess the property (P1). From the families listed in Section 4.1 possessing property (P1), it can be seen that only the following methods (listed in Tables 1–3) satisfy the condition (26). For all these methods $F_\infty \simeq 1.4 \times 10^{-2}\alpha^4 h^3$. It is interesting to note that the method in Table 2 is a limiting case ($\alpha_2 \to \frac{2}{3}$) of the family in Table 1 and further each of these two methods reduces to the classical two-stage third order Nyström method when y' is absent (Henrici [3]).

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TABLE 1. *Methods* $M_3(\alpha_2, 2/3; 1/4, -\alpha_2/6, 0)$.

α_i	β_{ij}	γ_{ij}	a_i	b_i
0			1/4	1/4
α_2	$-\alpha_2/6$	α_2	0	0
2/3	2/9 0	$2/3 - 2/9\alpha_2$ $2/9\alpha_2$	1/4	3/4

TABLE 2. *Method* $M_3^{(2)}(1/4, 3/4; -1/9, 0)$.

α_i	β_{ij}	γ_{ij}	a_i	b_i
0			1/4	1/4
2/3	-1/9	2/3	0	0
2/3	2/9 0	1/3 1/3	1/4	3/4

TABLE 3. *Method* $M_3^*(1/3; 0, -1/3)$.

α_i	β_{ij}	γ_{ij}	a_i	b_i
1/3			0	0
1/3	0	1/3	1/2	3/4
1	1 -1/3	-1 2	0	1/4

6. Numerical illustrations

In this section we illustrate numerically the performance of methods which satisfy the condition (26) as compared with the methods which do not satisfy (26). For the numerical experiments we selected two methods from the family $M_3(\alpha_2, \alpha_3; a_3; \beta_{21}, \beta_{32})$ corresponding to $\alpha_2 = \frac{1}{2}$, $\alpha_3 = 1$, $\beta_{21} = \beta_{32} = 0$, and we selected $a_3 = 0$ so that the method $M_3(\frac{1}{2}, 1; 0; 0, 0)$ satisfies (26) and $a_3 = \frac{1}{6}$ so that the method $M_3(\frac{1}{2}, 1; \frac{1}{6}; 0, 0)$ does not satisfy (26). These two methods were employed to solve the initial value problem:

$$y'' - 2y' + y = 0, \quad y(0) = 0, \quad y'(0) = 1, \tag{28}$$

whose exact solution is $y(x) = xe^x$. The numerical approximations obtained for y by these two methods and the corresponding relative errors F computed from (22) for a few values of h are shown in Table 4 at a few points x. The numerical experiments clearly demonstrate deterioration of the relative error for the method $M_3(\frac{1}{2}, 1; \frac{1}{6}; 0, 0)$, and confirm better performance of the method $M_3(\frac{1}{2}, 1; 0; 0, 0)$ which satisfies condition (26) over the method $M_3(\frac{1}{2}, 1; \frac{1}{6}; 0, 0)$ which does not satisfy condition (26).

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TABLE 4

	Method $M_3(\frac{1}{2}, 1; 0; 0, 0)$		Method $M_3(\frac{1}{2}, 1; \frac{1}{6}; 0, 0)$	
x	$\tilde{y}_n$	$10^4 F$	$\tilde{y}_n$	$10^4 F$
		$h = 0.2$		
5	0.74020307(3)	5	0.62623542(3)	339
10	0.21939975(6)	4	0.13871232(6)	462
15	0.48773357(8)	4	0.19642394(8)	610
20	0.96377719(10)	3	0.18960009(10)	816
25	0.17854262(13)	3	0.72351422(11)	1286
x	$\tilde{y}_n$	$10^5 F$	$\tilde{y}_n$	$10^5 F$
		$h = 0.1$		
5	0.74181119(3)	7	0.70607325(3)	994
10	0.22014674(6)	5	0.19246280(6)	1349
15	0.48999584(8)	5	0.37872502(8)	1722
20	0.96943792(10)	5	0.63465586(10)	2123
25	0.17981209(13)	4	0.94740906(12)	2568
x	$\tilde{y}_n$	$10^6 F$	$\tilde{y}_n$	$10^6 F$
		$h = 0.05$		
5	0.74203252(3)	9	0.74192272(3)	39
15	0.49030608(8)	6	0.48976659(8)	80
25	0.17998616(13)	6	0.17949815(13)	114
35	0.55499649(17)	6	0.55223319(17)	148

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