HIROSHIMA MATH. J.
12 (1982), 543–558

Modified Rosenbrock methods for stiff systems

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(Received April 23, 1982)

1. Introduction

Consider the initial value problem for a stiff system

(1.1) $$y' = f(y), \quad y(x_0) = y_0,$$

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

(1.2) $$x_j = x_0 + jh \qquad (j = 1, 2,\dots, h > 0),$$

and let $J(y)$ be the Jacobian matrix of $f(y)$. We are concerned with the case where approximations $y_j (j=1, 2,\dots)$ of $y(x_j)$ are computed by A-stable modified Rosenbrock methods of the form

(1.3) $$y_{n+1} = y_n + \textstyle\sum_{i=1}^{q} p_i k_i \qquad (n = 0, 1,\dots)$$

which require per step one evaluation of J, k evaluations of f and the solution of a system of m linear equations for q different right hand sides, where

(1.4) $$Mk_i = hf(y_n + \textstyle\sum_{j=1}^{i-1} a_{ij}k_j) + hJ \sum_{j=1}^{i-1} d_{ij}k_j \qquad (i = 1, 2,\dots, q),$$

the matrix $M = I - ahJ$ is nonsingular, $J = J(y_n + bhf(y_n))$, a and b are constants and $a > 0$.

Nørsett and Wolfbrandt [10] obtained an A-stable method of order 3 for $k = q = 2$. Kaps and Rentrop [6] have constructed an A-stable method of order 4 which embeds a method of order 3 for $k = 3$ and $q = 4$. Kaps and Wanner [7] have shown that there exists no A-stable method of order $k+1$ for $k = q = 4$, 5 and constructed an A-stable method of order k for $k = q = 5$, 6.

Bui [2] derived an L-stable method of order k for $k = q = 2$, 3, 4. Cash [4] has obtained a strongly A-stable method of order 3 which embeds a method of order 2 for $k = 2$ and $q = 4$. Artemev and Demidov [1] have proposed a variable order method which is A-stable and of order k for $k = 1$, 2, 3, 4.

The first object of this paper is to show that for $q = 2k+1$ $(k = 1, 2, 3)$ we can construct an A-stable modified Rosenbrock method of order $k+2$ and also a method of order $k+1$ by incorporating the first value of f in the next step of integration. The discrepancy of these two methods can be used for stepsize control. It is also shown that a strongly A-stable method of order $k+2$ exists for $k=1, 2, 3$. The second object of this paper is to show that there exists a variable order method which is A-stable and of order 2, 3, 5 for $k=1, 2, 3$ respectively. Finally these methods are illustrated by two numerical examples.

2. Preliminaries

Let

(2.1) $$f_1 = f(y_n),\quad J = J(y_n+bhf_1) \qquad (n \geqq 0)$$

and suppose that the matrix $M=I-ahJ$ $(a>0)$ is nonsingular, where a and b are constants. Let

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

(2.3) $t_{n+1} = t(x_n, y_n, y_{n+1}; h)$,

(2.4) $z_{n+1} = y_{n+1} + t_{n+1}$,

(2.5) $\Phi(x_n, y_n; h) = \sum_{j=1}^{k}(p_jk_j+q_jl_j)+rm_1+sn_1 \qquad (k = 1, 2, 3)$,

(2.6) $t(x_n, y_n, y_{n+1}; h) = \sum_{j=1}^{k}(p_j^*k_j+q_j^*l_j)+r^*m_1+s^*n_1+t^*hf^*$,

where $q_3=q_3^*=0$,

(2.7) $k_j=Kf_j$ $(j=1, 2, 3)$, $l_i=Lk_i$ $(i=1, 2)$, $m_1=Ll_1$, $n_1=Lm_1$, $f^*=f(y_{n+1})$,

$f_2=f(y_n+c_{21}k_1+d_{21}l_1)$, $f_3=f(y_n+\sum_{i=1}^{2}(c_{3i}k_i+d_{3i}l_i)+e_{31}m_1+g_{31}n_1)$,

(2.8) $K = hM^{-1}$, $L= KJ$, $M = I-ahJ$ $(a > 0)$,

c_{21}, d_{21}, c_{3i}, d_{3i}, q_i, q_i^* $(i=1, 2)$, p_j, p_j^* $(j=1, 2, 3)$, r, s, r^*, s^* and t^* are constants.

Let

(2.9) $u_2 = c_{21},\quad u_3 = c_{31}+c_{32},\quad X = u_2c_{32}+d_{31}+d_{32},$

$Y = d_{21}c_{32}+u_2d_{32}+e_{31},\quad Z = d_{21}d_{32}+g_{31},$

(2.10) $w_2 = u_2^2(c_{32}p_3+q_2),\quad w_3 = u_2^2d_{32}p_3,\quad b_1 = p_1+p_2+p_3,$

$b_2 = \sum_{i=2}^{3}u_ip_i+q_1+q_2,\quad b_3 = d_{21}p_2+Xp_3+u_2q_2+r,$

$b_4 = Yp_3+d_{21}q_2+s,\quad b_5 = Zp_3,$

(2.11) $p(a)=(2a-1)/2,\quad q(a)=(6a^2-6a+1)/6,\quad r(a)=(24a^3-36a^2+12a-1)/24,$

$s(a) = (120a^4-240a^3+120a^2-20a+1)/120,$

$t(a) = 720a^5-1800a^4+1200a^3-300a^2+30a-1,$

$u(a)=2a^2-4a+1,\quad v(a)=6a^3-18a^2+9a-1,$

$$w(a)=24a^4-96a^3+72a^2-16a+1,$$

$$z(a)=120a^5-600a^4+600a^3-200a^2+25a-1.$$

Replacing in (2.10) p_i $(i=1, 2, 3)$ and q_j $(j=1, 2)$ with p_i^* and q_j^* respectively, we define w_i^* $(i=2, 3)$ and b_j^* $(j=1, 2, 3, 4, 5)$. In the sequel for simplicity we impose the condition

(2.12) $$d_{21} = u_2(u_2-2a)/2, \quad X = u_3(u_3-2a)/2.$$

Let

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

(2.14) $$t(x; h) = t(x, y(x), y(x+h); h).$$

Then is Butcher's notation [3] $T(x; h)$ and $t(x; h)$ can be expanded into power series in h as follows:

(2.15) $$\begin{aligned} T(x; h) = {} & A_1hf+A_2(h^2/2)[f]+(h^3/3!)(A_3[_2f]_2+A_4[f^2]) \\ & +(h^4/4!)(B_1[_3f]_3+B_2[_2f^2]_2+B_3[[f]f]+B_4[f^3]) \\ & +(h^5/5!)(C_1[_4f]_4+C_2[_3f^2]_3+C_3[_2[f]f]_2+C_4[_2f^3]_2 \\ & +C_5[[_2f]_2f]+C_6[[f^2]f]+C_7[[f]^2]+C_8[[f]f^2]+C_9[f^4]) \\ & +(h^6/6!)(D_1[_5f]_5+D_2[_4f^2]_4+D_3[_3[f]f]_3+D_4[_3f^3]_3 \\ & +D_5[_2[_2f]_2f]_2+D_6[_2[f^2]f]_2+D_7[_2[f]^2]_2+D_8[_2[f]f^2]_2 \\ & +D_9[_2f^4]_2+D_{10}[[_3f]_3f]+D_{11}[[_2f^2]_2f]+D_{12}[[[f]f]f] \\ & +D_{13}[[f^3]f]+D_{14}[[_2f]_2[f]]+D_{15}[[f^2][f]]+D_{16}[[_2f]_2f^2] \\ & +D_{17}[[f^2]f^2]+D_{18}[[f]^2f]+D_{19}[[f]f^2]+D_{20}[f^4])+O(h^7), \end{aligned}$$

(2.16) $$t(x; h) = A_1^*hf+A_2^*(h^2/2)[f]+(h^3/3!)(A_3^*[_2f]_2+A_4^*[f^2])+\cdots.$$

For $k=1$ and $s=s^*=0$ we have

(2.17) $$A_1 = p_1-1,\ A_2 = 2(ap_1+q_1)-1, \quad A_3 = 6(r-q(a)+aA_2-a^2A_1),$$
$$A_4 = 3b(A_2+1)-1,$$

(2.18) $$B_1 = 24r(a)+12a(A_3-3aA_2+2a^2A_1), \quad B_2 = 4b(A_3+1)-1,\ B_3 = B_2-2,$$
$$B_4 = 2b(A_4+1)-1,$$

(2.19) $$A_1^*=p_1^*+t^*, \quad A_2^*=2(ap_1^*+q_1^*+t^*), \quad A_3^*=6(a^2p_1^*+2aq_1^*+r^*)+3t^*,$$
$$A_4^*=6b(ap_1^*+q_1^*)+3t^*,$$

(2.20) $$B_1^*=24a(a^2p_1^*+3aq_1^*+3r^*)+4t^*, \quad B_2^*=4(1-3b)t^*+4bA_3^*,$$
$$B_3^*=B_2^*+8t^*, \quad B_4^*=2bA_4^*+2(2-3b)t^*.$$

For $b=0$ we have

(2.21) $A_1=b_1-1,\quad A_2=2(b_2+p(a)+aA_1),\quad A_3=6(b_3-q(a)+aA_2-a^2A_1),$

$A_4=3\sum_{i=2}^{3} u_i^2 p_i-1,$

(2.22) $B_1=24(b_4+r(a))+12a(A_3-3aA_2+2a^2A_1),\quad B_2=12w_2+4a-1+4aA_1,$

$B_3=3B_4=12u_3^2(u_3-u_2)p_3+4u_2-3+4u_2A_4,$

(2.23) $C_1=120(b_5-s(a))+20a(B_1-6aA_3+12a^2A_2-6a^3A_1),$

$C_2=60w_3-20a^2+10a-1+10a(B_2-2aA_4),$

$C_3=3C_4=3(5a-1)-5(4a-1)u_2+5aB_3+5u_2(B_2-4aA_4),$

$C_5=120u_3Yp_3-2(20a^2-15a+2)+10a(B_3-4aA_4),\quad C_6=60u_3u_2^2c_{32}p_3-4,$

$C_8=2C_7=6C_9=-6+15(u_2+u_3)/2+10u_2u_3+5(u_2+u_3)B_3/2-10u_2u_3A_4,$

(2.24) $D_1=t(a)+30a(C_1-10aB_1+40a^2A_3-60a^3A_2+24a^4A_1),$

$D_2=120a^3-90a^2+18a-1+6a(3C_2-15aB_2+20a^2A_4),$

$D_4=D_3/3=120u_2w_3-30a^2+12a-1+2a(C_3-5aB_3),$

$D_5=720a(u_2-a)w_2+4(6a-1)+6aC_5,\quad D_6=4(6a-1)+6aC_6,$

$D_9=D_8/6=D_7/3=30u_2^2w_2+6a-1+2aC_7,$

$D_{10}=720u_3b_5+240a^3-270a^2+72a-5+6a(3C_5-15aB_3+40a^2A_4),$

$D_{11}=360u_3w_3+24a-5+6aC_6,\quad D_{13}=D_{12}/3=8u_2-5+2u_2C_6,$

$D_{14}=D_{16}=360u_3^2Yp_3-2(45a^2-36a+5)+6a(2C_8-5aB_3),$

$D_{15}=D_{17}=12u_3-10+3u_3C_6,\quad D_{19}=2D_{18}/3=10D_{20}=-10+12(u_2+u_3)$

$-15u_2u_3+2(u_2+u_3)C_8-5u_2u_3B_3,$

(2.25) $A_1^*=b_1^*+t^*,\ A_2^*=2(b_2^*+(1-a)t^*+aA_1^*),$

$A_3^*=6b_3^*+3u(a)t^*+6a(A_2^*-aA_1^*),\quad A_4^*=3(\sum_{i=2}^{3} u_i^2p_i^*+t^*),$

(2.26) $B_1^*=24b_4^*-4v(a)t^*+12a(A_3^*-3aA_2^*+2a^2A_1^*),$

$B_2^*=12w_2^*+4(1-3a)t^*+4aA_4^*,$

$B_3^*=3B_4^*=12u_3^2(u_3-u_2)p_3^*+12(1-u_2)t^*+4u_2A_4^*,$

(2.27) $C_1^*=120b_5^*+5w(a)t^*+20a(B_1^*-6aA_3^*+12a^2A_2^*-6a^3A_1^*),$

$C_2^*=60w_3^*+5(12a^2-8a+1)t^*+10a(B_2^*-2aA_4^*),$

$C_3^*=3C_4^*=5[3(1-4a)-5a(1-3a)u_2]t^*+5aB_3^*+5u_2(B_2^*-4aA_4^*),$

$C_5^*=120(u_3Yp_3^*+q(a)t^*)+10a(B_3^*-4aA_4^*),\quad C_6^*=6u_3u_2^2c_{32}p_3^*+20t^*,$

$C_8^*=2C_7^*=6C_9^*=30(1-u_2)(1-u_3)t^*+5(u_2+u_3)B_3^*-10u_2u_3A_4^*.$

The stability function of the method (2.2) for the test system $y'=\lambda y$ is given by

(2.28) $$R(z) = 1 + \sum_{j=1}^{5} b_j V^j$$

where $V=z/(1-az)$, $z=\lambda h$ and λ is an arbitrary complex number. Let $R(z)=P(z)/Q(z)$ and

(2.29) $$E(x) = |Q(ix)|^2 - |P(ix)|^2,$$

where i is the imaginary unit, and $P(z)$ and $Q(z)$ are polynomials in z. Then the method (2.2) is A-stable [9] if and only if

(2.30) $$E(x) \geqq 0 \qquad \text{for all real} \quad x.$$

Let $R(z)$ be the polynomial in V of exact degree p and

(2.31) $$P(z) = \sum_{j=0}^{p} e_j z^{p-j}, \quad Q(z) = (1-az)^p.$$

Then the method (2.2) is strongly A-stable if and only if $e_0=0$ and (2.30) is satisfied.

3. Construction of A-stable methods

In this section we shall show the following

THEOREM 1. *For* $k=1, 2, 3$ *there exists an A-stable method* (2.2) *of order* $k+2$ *and a method* (2.4) *of order* $k+1$; *a strongly A-stable method of order* $k+2$ *also exists.*

By this theorem the difference t_{n+1} of the methods (2.2) and (2.4) is available for stepsize control. If y_{n+1} is accepted as an approximation of $y(x_{n+1})$, then f^* can be used as f_1 in the next step of integration.

3.1. Case k=1

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

(3.1) $p_1=1,\ q_1=-p(a),\ \ r=q(a),\ \ b=1/3,\ \ B_1=24r(a),\ \ B_2=-B_4=1/3,$
$B_3 = -5/3,$

(3.2) $p_1^* = -t^*,\ \ q_1^* = (a-1)t^*,\ \ A_3^* = 6r^*+3u(a)t^*,\ \ A_4^* = t^*,$
$B_1^*=72ar^*+4(12a^3-18a^2+1)t^*,\ \ B_2^*=8r^*+4u(a)t^*,\ \ B_3^*=B_2^*+8t^*,$
$B_4^* = 8t^*/3,$

(3.3) $R(z) = 1 + V - p(a)V^2 + q(a)V^3.$

The equation $r(a)=0$ has three positive roots a_i $(i=1, 2, 3)$, where

(3.4) $$0 < a_1 < 1/6 < a_2 < 1/3,\ a_3 = 1.068579.$$

We consider first the case $q(a)\neq 0$. In this case we have

(3.5) $E(x) = c_1x^4 + c_2x^6, \quad e_0 = -v(a)/6,$

where

(3.6) $c_1 = -2r(a), c_2 = (3a-1)(6a-1)(v(a)+6a^3)/36.$

Hence the method (2.2) is A-stable if and only if $c_i \geqq 0$ $(i=1, 2)$, that is,

(3.7) $$1/3 \leqq a \leqq a_3.$$

The choice $a=1/3$, $r^*=7/432$ and $t^*=1/8$ yields

(3.8) $y_{n+1} = y_n + k_1 + l_1/6 - m_1/18,$

(3.9) $t_{n+1} = (hf^*-k_1)/8 - l_1/12 + 7m_1/432,$

(3.10) $B_1=-1/9, A_3^*=1/18, A_4^*=1/8, B_1^*=1/9, B_2^*=2/27, B_3^*=29/27, B_4^*=1/3.$

The method (2.2) is strongly A-stable if and only if $v(a)=0$ and (3.7) is satisfied, that is,

(3.11) $$a = 0.4358665215.$$

Choosing $r^*=17/400$ and $t^*=1/8$ for this value of a, we have

(3.12) $q_1=0.06413347849, \quad r=-0.07922023027, \quad B_1=-0.6215300316,$

(3.13) $p_1^*=-1/8, \quad q_1^*=-0.07051668481, \quad A_3^*=0.1186849362, \quad A_4^*=1/8,$
$B_1^*=0.6207694834, \quad B_2^*=0.1582465816, \quad B_3^*=1.1582465816, \quad B_4^*=1/3.$

Next we consider the case $q(a)=0$, namely $a=(3\pm\sqrt{3})/6$. Since

(3.14) $E(x) = (2a-1)^2(4a-1)x^4/4,$

the method (2.2) is A-stable if and only if $a\geqq 1/4$, so that we have

(3.15) $a = (3+\sqrt{3})/6, \quad B_1 = -(3+2\sqrt{3})/3,$

(3.16) $y_{n+1} = y_n + k_1 - \sqrt{3}l_1/6.$

The choice $r^*=0$ and $t^*=-1/16$ leads to

(3.17) $t_{n+1}=(k_1-hf^*)/16 + (3-\sqrt{3})l_1/96,$

(3.18) $A_3^* = (1+\sqrt{3})/6, \quad A_4^* = -1/16, \quad B_1^* = (3+2\sqrt{3})/6, \quad B_2^* = (1+\sqrt{3})/12,$
$B_3^* = -(5-\sqrt{3})/12, \quad B_4^* = -1/6.$

3.2. Case k=2

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

(3.19) $c_{21} = 3/4, \quad d_{21} = 3(3-8a)/32, \quad p_1 = 11/27, \quad p_2 = 16/27,$
$q_1 = -(22a+5)/54, \quad q_2 = 4(1-4a)/27, \quad r = (9a^2-a-1)/9,$
$s = -a(18a^2-19a+4)/18,$

(3.20) $C_1 = -120s(a), \quad C_2 = -20a^2+10a-1, \quad C_3 = 3C_4 = 3/4,$
$C_5 = -2(20a^2-15a+2), \quad C_6 = -4, \quad C_8 = 2C_7 = 6C_9 = -3/8,$

(3.21) $p_1^* = 7t^*/9, \; p_2^* = -16t^*/9, \; q_1^* + q_2^* = (3a+1)t^*/3, \; r^* + 3q_2^*/4 = 3(2-3a)t^*/3,$

(3.22) $B_1^* = 24(d_{21}q_2^* + s^*) - 4v(a)t^*, \; B_2^* = 27q_2^*/4 + 4(1-3a)t^*, \; B_3^* = 3B_4^* = 3t^*,$

(3.23) $C_1^* = 480a(d_{21}q_2^* + s^*) - 5(72a^4 - 192a^3 + 72a^2 - 1)t^*,$
$C_2^* = 135aq_2^*/2 + 5(1-12a^2)t^*, \quad C_4^* = C_3^*/3 = 135q_2^*/16 + 5(1-3a)t^*,$
$C_6^* = 20t^*, \quad C_8^* = 2C_7^* = 6C_9^* = 105t^*/8,$

(3.24) $R(z) = 1 + V - p(a)V^2 + q(a)V^3 - r(a)V^4.$

In the case $r(a) \neq 0$, we have

(3.25) $E(x) = c_3x^6 + c_4x^8, \quad e_0 = w(a)/24,$

where

(3.26) $c_3 = -(756a^5 - 1224a^4 + 768a^3 - 204a^2 + 24a - 1)/72,$

(3.27) $c_4 = (4a-1)(24a^2-12a+1)(w(a)+24a^4).$

Hence the method (2.2) is A-stable if and only if $c_i \geqq 0$ $(i=3, 4)$, that is,

(3.28) $$a_4 \leqq a \leqq a_5,$$

where

(3.29) $a_4 = (3+\sqrt{3})/12 = 0.394338, \quad a_5 = 1.28058.$

The choice $a = 2/5$, $q_2^* = 1/225$, $s^* = -1/1250$ and $t^* = 1/10$ yields

(3.30) $y_{n+1} = y_n + (11k_1 + 16k_2)/27 - 23l_1/90 + m_1/225 - 2(50l_2 - 9n_1)/1125,$

(3.31) $t_{n+1} = (7k_1 - 16k_2)/90 + 31l_1/450 + 11m_1/1500 + (50l_2 - 9n_1)/11250$
$+ hf^*/10,$

(3.32) $d_{21} = -3/160, \quad C_1 = 11/125, \quad C_2 = -1/5, \quad C_5 = 8/5,$

(3.33) $B_1^* = -157/2500, \quad B_2^* = -1/20, \quad B_3^* = 3B_4^* = 3/10, \; C_1^* = -259/1250,$
$C_2^* = -17/50, \quad C_3^* = 3C_4^* = -3/16, \quad C_5^* = 8/9, \quad C_6^* = 2, \quad C_8^* = 2C_7^* =$
$6C_9^* = 21/16.$

The method (2.2) is strongly A-stable if $w(a)=0$ and (3.28) is satisfied, namely

$$a = 0.5728160625. \tag{3.34}$$

Choosing $q_2^*=1/12$, $s^*=sq_2^*/q_2$ and $t^*=1/8$ in this case, we have

(3.35) $d_{21} = -0.1483620469, \quad q_1 = -0.3259620995, \quad q_2 = -0.1912984074,$

$r = 0.1533609012, \quad c = s/q_2 = -0.1625898283, \quad C_1 = 3.271078415,$

$C_2 = -1.834204204, \quad C_5 = 0.05975221696,$

(3.36) $p_1^*=7/72,\ p_2^*=-2/9,\ q_1^*=0.1132686745,\ q_2^*=1/12,\ r^*=-0.05578010831,$

$s^*=cq_2^*,$

$B_1^*=-0.3103660558, \quad B_2^*=0.2032759063, \quad B_3^*=3B_4^*=3/8,$

$C_1^*=-3.555653240, \quad C_2^*=1.386203541, \quad C_4^*=C_3^*/3=0.2540948828,$

$C_5^*=0.9775929186, \quad C_6^*=5/2, \quad C_8^*=2C_7^*=6C_9^*=105/64.$

Next we consider the case $r(a)=0$, that is, $a=a_1$, a_2 or a_3. Since $E(x)=c_2x^6$, by (3.6) the A-stability condition for (2.2) yields $a=a_3$,

$$C_1 = 3(20a^2-10a+1)/2 > 39/2, \quad C_2 = -2C_1/3 < -13,$$

$$C_5 = -(20a^2-15a+2) < -35/2.$$

Hence no useful method is obtained in this case.

3.3. Case k=3

Choosing $b=0$, $A_i=B_i=A_i^*=B_i^*=0$ $(i=1, 2, 3, 4)$ and $C_j=0$ $(j=1, 2,\dots, 9)$, we have

(3.37) $5(1-4a)u_2 = 3(1-5a), \quad u_3 = 1-a, \quad p_1+p_2+p_3 = 1,$

$u_2^2(u_2-u_3)p_2 = (3-4u_3)/12, \quad u_3^2(u_3-u_2)p_3 = (3-4u_2)/12,$

$15u_2u_3^2c_{32}p_3 = 1, \quad 60u_2^2d_{32}p_3 = 20a^2-10a+1,$

$60u_3Yp_3 = 20a^2-15a+2, \quad Zp_3 = s(a), \quad 12u_2^2(c_{32}p_3+q_2) = 1-4a,$

$u_2p_2+u_3p_3+q_1+q_2=-p(a), \quad d_{21}p_2+Xp_3+u_2q_2+r = q(a),$

$Yp_3+d_{21}q_2+s = -r(a),$

(3.38) $D_1=t(a),\ D_2=120a^3-90a^2+18a-1,\ D_4=D_3/3=2(1-5a)u_2+6a-1,$

$D_5 = -2D_{14} = -2D_{16} = 4(60a^3-60a^2+15a-1),$

$D_6=-2D_{15}=-2D_{17}=4(6a-1),\ D_8=2D_7=6D_9=9(1-5a)u_2+6(6a-1),$

$D_{10} = 240a^3-270a^2+72a-5+720u_3s(a),$

$$D_{11} = -120a^3+180a^2-42a+1, \quad D_{13} = D_{12}/3 = 8u_2-5,$$
$$D_{19} = 2D_{18}/3 = 10D_{20} = 5u_3^2(3-4u_2)+12u_2-10,$$

(3.39) $p_1^*+p_2^*+p_3^*+t^*=0,\ u_2^2(u_2-u_3)p_2^*=(u_3-1)t^*,\ u_3^2(u_3-u_2)p_3^*=(u_2-1)t^*,$
$5u_3u_2^2q_2^* = (1-5a^2)t^*, \quad u_2p_2^*+u_3p_3^*+q_1^*+q_2^*+(1-a)t^*=0,$
$d_{21}p_2^*+Xp_3^*+u_2q_2^*+r^*+u(a)t^*/2=0,\ Yp_3^*+d_{21}q_2^*+s^*-v(a)t^*/6=0,$

(3.40) $C_1^*=5[96(5a-2)s(a)+w(a)]t^*, \quad C_2^*=(400a^3-300a^2+60a-3)t^*,$
$C_3^*=3C_4^*=5[3(1-4a)-4(1-3a)u_2]t^*,\ C_5^*=4(200a^3-200a^2+50a-3)\,t^*,$
$C_6^*=4(20a-3)t^*, \quad C_8^*=2C_7^*=6C_9^*=30a(1-u_2)t^*,$

(3.41) $R(z) = 1 + V - p(a)V^2 + q(a)V^3 - r(a)V^4 + s(a)V^5.$

If $(1-a)(1-4a)(1-5a)\neq 0$, from (3.37) c_{21}, d_{21}, c_{3i}, d_{3i}, q_i $(i=1, 2)$, e_{31}, g_{31}, p_j $(j=1, 2, 3)$, r and s are determined uniquely for given a.

In the case $s(a)\neq 0$, we have

(3.42) $E(x) = c_5x^6-2c_6x^8+c_7x^{10}, \quad e_0 = -z(a)/120,$

where

(3.43) $c_5 = (720a^5-1800a^4+1200a^3-300a^2+30a-1)/360,$

(3.44) $c_6=(57600a^7-158400a^6+144960a^5-63600a^4+14880a^3-1880a^2$
$+120a-3)/57600,$

(3.45) $c_7 = (120a^5+z(a))\,(120a^5-z(a)).$

The method (2.2) is A-stable if and only if $c_5\geqq 0$, $c_7\geqq 0$ and $c_6\leqq\sqrt{c_5c_7}$, that is,

(3.46) $a_6 \leqq a \leqq a_7 \quad \text{or} \quad a_8 \leqq a \leqq a_9,$

where

(3.47) $a_6 = 0.24651, \quad a_7 = 0.36180, \quad a_8 = 0.42078, \quad a_9 = 0.47326.$

The choice $a=1/3$ and $t^*=1/12$ yields

(3.48) $c_{21} = 6/5, \quad d_{21} = 8/25, \quad c_{31} = 406/729, \quad c_{32} = 80/729,$
$d_{31} = -2552/19683, \quad d_{32} = -40/19683, \quad e_{31} = -416/6561,$
$g_{31} = 80/19683,$

(3.49) $y_{n+1} = y_n+(1144k_1+125k_2+2187k_3)/3456-(272l_1+115l_2)/1296$
$+17m_1/432+17n_1/324,$

(3.50) $t_{n+1} = (80k_1-125k_2-243k_3)/3456+(35l_1+10l_2)/1296+m_1/144$
$-n_1/648+hf^*/12,$

(3.51) $D_1 = 23/27, \quad D_2 = -5/9, \quad D_3 = 3D_4 = -9/5,$

$D_5 = -2D_{14} = -2D_{16} = -16/9, \quad D_6 = 4, \quad D_8 = 2D_7 = 6D_9 = -6/5,$

$D_{10} = -29/27, \quad D_{11} = 23/9, \quad D_{12} = 3D_{13} = 69/5, \quad D_{15} = D_{17} = -2,$

$D_{19} = 2D_{18}/3 = 10D_{20} = 2/5,$

(3.52) $C_1^* = 137/972, \quad C_2^* = -41/324, \quad C_3^* = 3C_4^* = -5/12, \quad C_5^* = -31/81,$

$C_6^* = 11/9, \quad C_8^* = 2C_7^* = 6C_9^* = -1/6,$

(3.53) $D_1^* = 583/486, \quad D_2^* = -29/54, \quad D_3^* = 3D_4^* = -157/90, \quad D_5^* = -58/9,$

$D_6^* = 10/9, \quad D_8^* = 2D_7^* = 6D_9^* = 181/15, \quad D_{10}^* = -1037/486,$

$D_{11}^* = 269/162, \quad D_{12}^* = 3D_{13}^* = 43/10, \quad D_{14}^* = D_{16}^* = -161/81,$

$D_{15}^* = D_{17}^* = 37/9, \quad D_{19}^* = 2D_{18}^*/3 = 10D_{20}^* = -43/45.$

The method (2.2) is strongly A-stable if $z(a)=0$ and (3.46) is satisfied, that is,

(3.54) $$a = 0.2780538411.$$

For this value of a we have

(3.55) $c_{21} = 2.086715347, \quad d_{21} = 1.596971253, \quad c_{31} = 0.6880907035,$

$c_{32} = 0.03385545541, \quad d_{31} = -0.009352040051,$

$d_{32} = -0.001431432753, \quad e_{31} = -0.07409613665,$

$g_{31} = 0.005937857065,$

(3.56) $p_1 = 0.3720306131, \quad p_2 = 0.001573567760, \quad p_3 = 0.6263958192,$

$q_1 = -0.2102070122, \quad q_2 = -0.02335447252, \quad r = -0.02535011637,$

$s = 0.04882735273,$

(3.57) $D_1 = 0.3816347293, \quad D_2 = -0.3735928198,$

$D_4 = D_3/3 = -0.9604384354,$

$D_5 = -2D_{14} = -2D_{16} = -0.7127297665,$

$D_6 = -2D_{15} = -2D_{17} = 2.673292187,$

$D_7 = D_8/2 = 3D_9 = -1.659744195, \quad D_{10} = 0.4935616656,$

$D_{11} = 0.6585551038, \quad D_{12} = 3D_{13} = 35.08116834,$

$D_{19} = 2D_{18}/3 = 10D_{20} = 1.106496130.$

The choice $t^* = 1/8$ yields

(3.58) $p_1^* = 0.07181502854,\quad p_2^* = -0.005848618348,\quad p_3^* = -0.1909664102,$

$q_1^* = 0.05495023631,\quad q_2^* = 0.004878361809,\quad r^* = 0.007941406168,$

$s^* = 0.007189851420,\quad t^* = 0.125,$

(3.59) $C_1^* = 0.03971741473,\quad C_2^* = -0.1139970082,$

$C_3^* = 3C_4^* = -1.075548044,\quad C_5^* = -0.1303043710,$

$C_6^* = 1.280538411,\quad C_8^* = 2C_7^* = 6C_9^* = -1.133120162,$

(3.60) $D_1^* = 0.3313073918,\quad D_2^* = -0.4369146771,$

$D_4^* = D_3^*/3 = -1.073879143,\quad D_5^* = -10.52551645,$

$D_6^* = 0.9655441270,\quad D_7^* = D_8^*/2 = 3D_9^* = 28.12658147,$

$D_{10}^* = -1.274483999,\quad D_{11}^* = 2.024902351,$

$D_{12}^* = 3D_{13}^* = -4.018015275,\quad D_{14}^* = D_{16}^* = -4.489377832,$

$D_{15}^* = D_{17}^* = 4.858843171,\quad D_{19}^* = 2D_{18}^*/3 = 10D_{20}^* = -8.631342287.$

Finally we consider the case $s(a)=0$. Since we have (3.25) in this case, the A-stability condition for (2.2) is given by (3.28). The equation $s(a)=0$ has four positive roots r_i $(i=1, 2, 3, 4)$, where

$$r_1 = 0.09129,\quad r_2 = 0.17448,\quad r_3 = 0.38886,\quad r_4 = 1.34537.$$

These roots do not satisfy the condition (3.28), so that no A-stable method exists in this case.

4. A variable order method

In this section we consider only the case $b=0$ and show the following

THEOREM 2. *For $k=3$ there exist a method* (2.4) *of order* 4 *and an A-stable method* (2.2) *of order* 5 *which embeds an A-stable method of order $j+1$ $(j=1, 2)$ with j function evaluations.*

Let

(4.1)$_j$ $\quad y_{n+1}^j = y_n + \Phi_j(x_n, y_n; h) \quad (j = 2, 3, 5),$

(4.2) $\quad y_{n+1}^4 = y_n + \Psi(x_n, y_n, y_{n+1}; h),$

(4.3) $\quad \Phi_j(x_n, y_n; h) = \sum_{i=1}^k (p_i^j k_i + q_i^j l_i) + r^j m_1 + s^j n_1$

$$(j = (k^2 - k + 1)/2,\ k=1, 2, 3),$$

(4.4) $\quad \Psi(x_n, y_n, y_{n+1}^5; h) = \sum_{i=1}^3 (p_i^4 k_i + q_i^4 l_i) + r^4 m_1 + s^4 n_1 + t^4 hf^*,$

where

(4.5) $\quad q_3^j = 0\ (j=2, 3, 4, 5), \quad q_2^3 = r^2 = s^2 = s^3 = 0, \quad f^* = f(y_{n+1}^5).$

Let

(4.6) $\quad T_j(x; h) = y(x) + \Phi_j(x, y(x); h) - y(x+h) \qquad (j = 2, 3, 5),$

(4.7) $\quad T_4(x; h) = y(x) + \Psi(x, y(x), y(x+h); h) - y(x+h).$

Then $T_j(x; h)$ $(j=2, 3, 4, 5)$ can be expanded into power series in h as follows:

(4.8) $\quad T_j(x; h) = A_1^j hf + A_2^j(h^2/2)[f] + (h^3/3!)(A_3^j[_2f]_2 + A_4^j[f^2]) + \cdots.$

The condition $A_i^2=0$ $(i=1, 2)$ yields (3.14) and

(4.9) $$p_1^2 = 1, \quad q_1^2 = -p(a).$$

For this choice of parameters the method $(4.1)_2$ is of order 2 and is A-stable if and only if $a \geqq 1/4$.

The choice $A_i^3=0$ $(i=1, 2, 3, 4)$ leads to (3.5) and

(4.10) $\quad p_1^3 + p_2^3 = 1, \quad u_2 p_2^3 + q_1^3 = -p(a), \quad d_{21}p_2^3 + r^3 = q(a), \quad u_2^2 p_2^3 = 1/3.$

If $u_2 \neq 0$, from (4.10) p_i^3 $(i=1, 2)$, q_1^3 and r^3 are determined uniquely for any given a and d_{21} and the method $(4.1)_3$ is of order 3. It is A-stable if and only if (3.7) is satisfied.

The condition $A_i^5=B_i^5=0$ $(i=1, 2, 3, 4)$ and $C_j^5=0$ $(j=1, 2, \ldots, 9)$ yields (3.37) and (3.42). If $(1-a)(1-4a)(1-5a) \neq 0$, then $u_2u_3(u_3-u_2) \neq 0$ and from (3.37) c_{21}, d_{21}, c_{3i}, d_{3i}, q_i^5 $(i=1, 2)$, e_{31}, q_{31}, p_j^5 $(j=1, 2, 3)$, r^5 and s^5 are determined uniquely for any given a and the method $(4.1)_5$ is of order 5. It is A-stable if and only if (3.46) is satisfied.

Thus the methods $(4.1)_j$ $(j=2, 3, 5)$ are A-stable together if and only if

(4.11) $$1/3 \leqq a \leqq a_7 \quad \text{or} \quad a_8 \leqq a \leqq a_9.$$

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

(4.12) $$\begin{aligned} &u_2^2(u_2-u_3)p_2^4+(1-u_3)t^4=(3-4u_3)/12, \quad d_{21}p_2^4+Xp_3^4+r^4+u(a)t^4/2=q(a),\\ &\textstyle\sum_{i=1}^3 p_i^4+t^4=1, \quad 12u_2^2(c_{32}p_3^4+q_2^4)+4(1-3a)t^4=1-4a,\\ &u_2p_2^4+u_3p_3^4+q_1^4+q_2^4+(1-a)t^4=-p(a),\\ &u_3^2(u_3-u_2)p_3^4+(1-u_2)t^4=(3-4u_2)/12, \quad Yp_3^4+d_{21}q_2^4+s^4-v(a)t^4/6=-r(a). \end{aligned}$$

If $u_2u_3(u_3-u_2) \neq 0$, from these p_j^4 $(j=1, 2, 3)$, q_i^4 $(i=1, 2)$, r^4 and s^4 are determined uniquely for any given a, d_{21}, c_{32}, u_2, u_3, X, Y and t^4, and the method (4.2) is of order 4.

Taking into consideration (4.11) and the condition $(1-a)(1-4a)(1-5a)\neq 0$, we choose

(4.13) $$a = 1/3, \quad t^4 = 1/12.$$

Then it follows that

(4.14) $y_{n+1}^2 = y_n + k_1 + l_1/6,$

(4.15) $A_3^2 = 1/3, \quad A_4^2 = -1, \quad B_1^2 = 11/9, \quad B_2^2 = -1, \quad B_3^2 = 3B_4^2 = -3,$

(4.16) $c_{21} = 6/5, \quad d_{21} = 8/25,$

(4.17) $y_{n+1}^3 = y_n + (83k_1 + 25k_2)/108 - l_1/9 - 7m_1/54,$

(4.18) $B_1^3 = -1/9, \quad B_2^3 = 1/3, \quad B_3^3 = 3B_4^3 = 9/5,$

(4.19) $c_{31} = 406/729, \quad c_{32} = 80/729, \quad d_{31} = -40/19683,$
$d_{32} = -2552/19683, \quad e_{31} = -416/6561, \quad g_{31} = 80/19683,$

(4.20) $y_{n+1}^5 = y_n + (1144k_1 + 125k_2 + 2187k_3)/3456 - (272l_1 + 115l_2)/1296$
$+17m_1/432 + 17n_1/324,$

(4.21) $y_{n+1}^4 = y_n + (17k_1 + 27k_3 + 4hf^*)/48 - (474l_1 + 205l_2)/2592$
$+ 5m_1/108 + 11n_1/216,$

(4.22) $C_1^4 = 137/972, \quad C_2^4 = -41/324, \quad C_3^4 = 3C_4^4 = -5/12, \quad C_5^4 = -31/81,$
$C_6^4 = 11/9, \quad C_8^4 = 2C_7^4 = 6C_9^4 = -1/6.$

5. Numerical examples

Numerical results on two problems are presented in this section.

Problem 1. $y' = -By + Uw, \ y(0) = -(1, 1, 1, 1)^T,$
where

(5.1) $y = Uz, \quad z = (z_1, z_2, z_3, z_4)^T, \quad w = (z_1^2, z_2^2, z_3^2, z_4^2)^T,$
$U = (u_{ij}), \quad u_{ij} = 1/2 \ (i \neq j), \quad u_{ii} = -1/2 \ (i, j = 1, 2, 3, 4),$
$B = UDU, \quad D = \mathrm{diag}(\beta_1, \beta_2, \beta_3, \beta_4), \quad \beta_1 = 1000, \quad \beta_2 = 800,$
$\beta_3 = -10, \quad \beta_4 = 0.001.$

The exact solution given in [5] is

(5.2) $y(x) = Uz(x), \quad z_i(x) = \beta_i/(1+c_i e^{\beta_i x}), \quad c_i = -(1 + \beta_i) \quad (i = 1, 2, 3, 4).$

Problem 2. $y' = Ay, \ y(0) = (2, 1, 2)^T,$
where

(5.3) $A = (a_{jj}),\quad a_{11} = -0.1,\quad a_{12} = -49.9,\quad a_{22} = -50,\quad a_{32} = 70,$
$a_{33} = -120,\quad a_{13} = a_{21} = a_{23} = a_{31} = 0,\quad y = (y_1, y_2, y_3)^T.$

The exact solution given in [8] is

(5.4) $$y_1(x) = e^{-0.1x} + e^{-50x},\quad y_2(x) = e^{-50x},\quad y_3(x) = e^{-50x} + e^{-120x}.$$

To avoid the multiplication of the matrix J by a vector g, the vector $v=Lg$ is obtained by the formula $M(v+g/a)=g/a$, because $L=KJ=(M^{-1}-I)/a$ by (2.8). The matrix M is decomposed by LU-factorization and the infinity norm is used.

For methods (3.8), (3.30) and (3.49) computation is carried out in the following manner:

(1) Compute y_1, t_1, $d=\|t_1\|$ and $r=\max(1, \|y_1\|)$.
(2) If $d>\varepsilon r$, then halve the stepsize; replace δ by $\delta/8$ if $w=1$; go to (1).
(3) Replace x_0 and y_0 by x_1 and y_1 respectively and set $w=0$.
(4) If $d<\delta r$, then double the stepsize and set $w=1$.
(5) Go to (1).

Initially $h=1/64$, $\varepsilon=10^{-2}/2$, $\delta=2^{-k-4}\varepsilon$ $(k=1, 2, 3)$ and $w=0$. The error e and the number s of integration steps are listed in Table 1.

The program for the variable order method is as follows:

(1) Compute y_1^2, y_1^3, $d=\|y_1^3-y_1^2\|$ and $r=\max(1, \|y_1^3\|)$.
(2) If $d\leqq\varepsilon r$, then set $y_1=y_1^3$ and go to (6).
(3) Compute y_1^5, y_1^4, $d=\|y_1^5-y_1^4\|$ and $r=\max(1, \|y_1^5\|)$.
(4) If $d\leqq\varepsilon r$, then set $y_1=y_1^5$ and go to (6).
(5) Halve the stepsize; replace δ by $\delta/8$ if $w=1$; go to (1).
(6) Replace x_0 and y_0 by x_1 and y_1 respectively and set $w=0$.
(7) If $d\leqq\delta r$, then double the stepsize and set $w=1$.
(8) Go to (1).

Initially $h=1/64$, $\varepsilon=10^{-2}/2$, $\delta=2^{-5}\varepsilon$ and $w=0$. The error e, the number s of integration steps and the number n of steps in which the method of order 5 is not used are listed in Table 2.

Table 1.

Prob	x	$k=1$		$k=2$		$k=3$	
		e	s	e	s	e	s
1	1/64	1.614E–2	10	6.619E–3	8	3.595E–3	6
	1/8	6.975E–2	25	6.144E–2	16	9.850E–2	12
	1	4.628E–3	88	1.822E–3	62	1.139E–2	21
	8	3.401E–3	144	2.668E–3	84	4.524E–3	30
2	1/64	5.502E–4	2	9.772E–5	5	3.903E–3	1
	1/8	9.228E–3	10	6.482E–4	12	9.291E–4	6
	1	2.228E–2	19	8.978E–3	21	7.050E–3	12
	8	4.769E–2	29	3.814E–2	30	3.054E–2	18

Table 2.

x	Problem 1			Problem 2		
	e	s	n	e	s	n
1/64	8.279E–3	7	5	3.903E–3	1	0
1/8	7.243E–2	17	14	9.570E–6	8	6
1	1.495E–2	38	34	1.652E–2	17	15
8	1.342E–2	47	43	4.097E–2	26	22

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