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Efficient Explicit Runge-Kutta Methods for Stiff Systems

By

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Abstract

We study the explicit Runge-Kutta methods for stiff-equation $y'=\lambda y$, where the methods are variable coefficients formulas depending on λ. They are A-stable with respect to the model equation $y'=\lambda y$. The analysis of eigenvalue λ for some schemes are carried out. Finally, some numerical tests justifing the results are present.

1. Introduction

The present paper is concerned with the numerical integration of stiff system of ordinary differential equation:

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

A basic difficulty in the numerical solution of stiff system is the satisfying of the requirement of stability. From the restriction of stability, implicit type methods have been present and some explicit methods imposed the stability conditions have derived, however, there still remain stability problem for the explicit methods, so it is the purpose of the present paper to derive the explicit A-stable Runge-Kutta methods with respect to the model equation. The outline of this paper is as follows: In §2, We consider two-stage of order one, three-stage of order two and four-stage of order three explicit A-stable Runge-Kutta methods for the fitting problem respectively. Stability analysis for arbitrary eigenvalue λ are discussed in §3. In §4, we propose some numerical tests.

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2. Derivation of the formulae

Consider the r-stage explicit Runge-Kutta methods:

$$\begin{aligned} y_{n+1} &= y_n + h\sum_{i=1}^{r} b_i k_i, \qquad (2.1)\\ k_1 &= f(x_n, y_n),\\ k_i &= f(x_n+c_i h, y_n+h\sum a_{ij} k_j),\\ &\quad c_i = \sum_i a_{ij} \quad (i=2, \ldots, r). \end{aligned}$$

The order conditions of the R-K methods which are discussed in [1], are listing up to three order:

order 1: $\sum_i b_i = 1,$ (2.2)

order 2: $\sum_i b_i c_i = 1/2,$ (2.3)

order 3: $\sum_i b_i c_i = 1/3,$ (2.4)

$\sum_i b_i a_{ij} c_j = 1/6.$

Let us now apply the r-stage, p-th order Runge-Kutta methods (2.1) to the test equation

$$y' = \lambda y, \qquad (2.5)$$

then we have

$$y_{n+1} = S(z) y_n, \qquad (2.6)$$

and $S(z)$ takes the form:

$$S(z) = \sum_{i=1}^{p} \frac{z^i}{i!} + \sum_{\kappa=p+1}^{r} \gamma_\kappa z^\kappa, \quad (z=\lambda h)$$

where γ are the function of the coefficients of (2.1).

we shall study how the function $S(z)$ of (2.6) with $(p, r) = (1, 2)$, $(2, 3)$ and $(3, 4)$ are expressed.

Case (1) $p=1$, $r=2$: From (2.6) we obtain the difference equation:

$$y_{n+1} = (1+z+b_2 a_{21} z^2) y_n, \qquad (2.7)$$

here if we take $b_2 a_{21}$ in the form:

$$b_2 a_{21} = \frac{\delta}{\alpha+\beta z}, \qquad (2.8)$$

then from (2.7) and (2.8) we have

$$y_{n+1} = \frac{\alpha + (\alpha+\beta) z + (\beta+\delta) z^2}{\alpha+\beta z} y_n . \tag{2.9}$$

From the stability condition, we have $\beta+\delta=0$, taking, for example, $\alpha=1$, $\beta=-1$ we have

$$y_{n+1} = \frac{1}{1-z} y_n , \tag{2.10}$$

which is A-stable algorithm. Solving (2.8) with $\alpha=1$, $\beta=-1$ and the order condition (2.2), we have

$$b_2 = \frac{1}{c_2(1-z)} ,\ b_1 = 1-b_2 . \tag{2.11}$$

(c_2: free parameter)

Case (11) $p=2$, $r=3$: Proceeding the same way as the case (1), we have

$$y_{n+1} = \left(1+z+\frac{z^2}{2!}+b_3\, a_{32}\, a_{21}\, z^{3}_{21}\right) y_n , \tag{2.12}$$

setting

$$b_3\, a_{32}\, a_{21} = \frac{\gamma}{2!\,(\alpha+\beta z)} , \tag{2.13}$$

we have

$$y_{n+1} = \frac{2\alpha + 2(\alpha+\beta) z + (2\beta+\alpha) z^2 + (\beta+\gamma) z^3}{2!\,(\alpha+\beta z)} y_n .$$

From the stability condition, we have

$$2\beta+\alpha = 0,\ \beta+\gamma = 0,$$

which lead to the following A-stable algorithm:

$$y_{n+1} = \frac{2+z}{2-z} y_n . \tag{2.14}$$

Solving (2.13) and order conditions (2.2) and (2.3), we have

$$b_3 = -\frac{1}{2!\, a_{32}\, a_{21}\,(2-z)},\ b_2 = \frac{1}{c_2}\left(\frac{1}{2} - b_3\, c_3\right), \tag{2.15}$$
$$a_{21} = c_2,\ a_{31} = c_3 - a_{32},$$
$$b_1 = 1 - (b_2 + b_3).\quad (c_2,\ c_3,\ a_{32}\text{: free parameter})$$

Case (III) $p=3$, $r=4$: Finally in this section, we concern four-stage three order method, integrating (2.5), we have

$$y_{n+1} = \left(1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + b_4\, a_{43}\, a_{32}\, a_{21}\, z^4\right) y_n, \tag{2.16}$$

here we set

$$b_4\, a_{43}\, a_{32}\, a_{21} = \frac{\gamma}{3!\,(\alpha + \beta z)}, \tag{2.17}$$

putting (2.17) into (2.16), we have

$$y_{n+1} = \frac{6\alpha + 6(\alpha+\beta) z + (6\beta + 3\alpha) z^2 + (3\beta + \alpha) z^3 + (\beta + \gamma) z^4}{3!\,(\alpha + \beta z)} y_n.$$

From the stability condition, we have

$$6\beta + 3\alpha = 0,\ 3\beta + \alpha = 0,\ \beta + \gamma = 0,$$

which lead to

$$\alpha = \beta = 0.$$

It follows that the assupution (2.17) is unsuitable. We now consider the following further case:

$$b_4\, a_{43}\, a_{32}\, a_{21} = \frac{\delta + \rho z}{3!\,(\alpha + \beta z + \gamma z^2)}, \tag{2.18}$$

putting (2.18) into (2.16), we have

$$y_{n+1} = \frac{u}{3!\,(\alpha + \beta z + \gamma z^2)} y_n,$$

with

$$u=6\alpha+6(\alpha+\beta)z+(6\gamma+6\beta+3\alpha)z^2+(6\gamma+3\beta+\alpha)z^3$$
$$+(3\gamma+\beta+\delta)z^4+(\gamma+\rho)z^5.$$

From the stability condition we have

$$\gamma+\rho=0,\ 3\gamma+\beta+\delta=0,\ 6\gamma+3\beta+\alpha=0,$$

which lead to

$$\alpha=3\delta-3\rho,\ \beta=3\rho-\delta,\ \gamma=-\rho. \tag{2.19}$$

If we take $\delta=1$, $\rho=-1$ in (2.19), we have following L-stable algorithm:

$$y_{n+1}=\frac{6+2z}{6-4z+z^2}y_n. \tag{2.20}$$

Solving (2.18) and order conditions (2.2), (2.3), (2.4), we have

$$\begin{aligned}
b_4&=\frac{1}{a_{43}\,a_{32}\,a_{21}}\,\frac{1-z}{6-4z+z^2}, \qquad (2.21)\\
b_2&=\frac{1}{c_2(c_3-c_2)}\left\{\frac{1}{2}(1-b_4\,c_4)\,c_3-\frac{1}{3}+b_4\,c_4^2\right\},\\
b_3&=\frac{1}{c_3}\left\{\frac{1}{2}-b_4\,c_4-b_2\,c_2\right\},\\
a_{42}&=\frac{1}{b_4\,c_2}\left\{\frac{1}{6}-b_3\,a_{32}\,c_2-\frac{c_3}{c_2}a_{43}\right\},\\
a_{21}&=c_2,\ c_3=b_{31}+b_{32},\ a_4=c_4-(a_{42}+a_{43}).
\end{aligned}$$

(a_{32}, a_{31}, a_{43}, c_2, c_4: free parameters).

3. Stability properties of the schemes (2.11), (2.15) and (2.21)

In this section we are concerned with the analysis of eigenvalue of schemes (2.10), (2.14) and (2.20). Let us set λ' be the approximation of λ, replacing z by $z'=\lambda' h$ in (2.8), the algorithm (2.10) is then

$$y_{n+1}=\left(1+z+\frac{z^2}{1-z'}\right)y_n,$$

or

$$\begin{aligned}
y_{n+1}&=\pi(z,z')\,y_n,\\
\pi(z,z')&=1+z+\frac{z^2}{1-z'}, \qquad (3.1)
\end{aligned}$$

we may write (3.1) in the form

$$\pi(z, z') = \left(\frac{1}{1-z} + \frac{z^2}{1-z'} - \frac{z^2}{1-z}\right), \tag{3.2}$$

so if z' satisfies the equation

$$\left| z^2\left(\frac{1}{1-z'} - \frac{1}{1-z}\right)\right| < 1 - \left|\frac{1}{1-z}\right|, \tag{3.3}$$

then the algorithm (3.1) is A-stable. Setting $z = re^{i\theta}(\pi/2 < \theta < 3\pi/2)$, and using the inequality

$$|1-z| < 1+r,$$

in (3.3), we have

$$\left|\frac{z'-z}{z'-1}\right| < \frac{1}{r+2},$$

which lead to the following result.

Theorem 1. *The algorithm (2.11) with $z=z'$ is A-stable if z' satisfies the inequality*:

$$\left|\frac{z'-z}{z'-1}\right| < \frac{1}{r+2}. \tag{3.4}$$

The region z' satisfying (3.4) lies in the interior of the circle with the center m_1 and the radius r_1,

$$m_1 = -\frac{c^2-z}{1-c^2}, \quad r_1 = c\frac{|1-z|}{1-c^2}, \tag{3.5}$$

with $c = 1/(r+2)$. Taking the value of r large enough, we have the following result:

Corollary. *For large value of z, the algorithm (2.11) with $z=z'$ is A-stabe if z' satisfies the inequality*:

$$|z-z'| < 1.$$

Carring the same argument to the algorithm (2.15) and (2.21), we have the following results:

Theorem 2. *The algorithm (2.15) with $z=z'$ is A-stable if z' satisfies the inequality*:

$$\left|\frac{z'-z}{z'-2}\right|<\frac{2}{r^3}(\sqrt{z_1}-\sqrt{z_2}). \tag{3.6}$$

with

$$z_1 = r^2-4r\cos(\theta)+4,$$
$$z_2 = r^2+4r\cos(\theta)+4,$$

The region z' satisfing (3.6) is in the interior of the circle with the center m_2 and the radius r_2

$$m_2 = -\frac{c^2-z}{1-c^2}, \quad r_2 = c\left|\frac{2-z}{1-c^2}\right|, \tag{3.7}$$

with $c=2(\sqrt{z_1}-\sqrt{z_2})/r^3$.

Theorem 3. *The algorithm (2.21) with $z=z'$ is A-stable if z' satisfies the following inequality*:

$$\left|\frac{(z-z')(zz'-(z+z')-2)}{(6-4z'+z'^2)(6-4z+z^2)}\right|<\frac{6}{|z^4|}\left\{1-\frac{|6+2z|}{|6-4z+z^2|}\right\}.$$

4. Numerical Examples

In order to test the method (2.1), we wish to present some numerical results. The described methods are programmed in FORTRAN and run on the Personal Computer 9801RA (NEC). The computations are done in double precision.

(1) $y'=-1000y$, $y(0)=1$,

(2) $Y'=AY$, $Y(0)=(1,1,1)$,

with

$$A=\begin{pmatrix} -0.1 & 0 & 0 \\ 0 & -50 & 0 \\ 0 & 0 & -120 \end{pmatrix},$$

(3) $Y'=AY$, $Y(0)=(1,1,1)$,

with

$$A=\begin{pmatrix} 0.1 & 0 & 0 \\ 0 & -50 & 0 \\ 0 & 0 & -120 \end{pmatrix},$$

Table 1

Result using (2.11) with $h=1/2^3$ and $1/2^6$.

Problem 1

Absolute error

x	0.125	0.500..	1
$h=1/2^3$	$0.793E-2$	$0.396E-8$	$0.157E-16$
$h=1/2^6$	$0.171E-9$	0	0

Comparison with the methods order 1 (2.11), order 2 (2.15) and order 3 (2.21).

($h=1/2^3$)

Absolute error

x	0.125	0.5	1
order 1 (2.11)	$0.793E-2$	$0.396E-8$	$0.157E-16$
order 2 (2.15)	$0.968E0$	$0.879E0$	$0.774E0$
order 3 (2.21)	$0.248E-1$	$0.379E-6$	$0.1443E-12$

Problem 2

($h=1/2^6$)

Absolute error

$x=0.0625$	y_1	y_2	y_3
order 1 (2.11)	$0.484E-5$	$0.553E-1$	$0.140E-1$
order 2 (2.15)	$0.126E-8$	$0.706E-2$	$0.552E-3$
order 3 (2.21)	$0.329E-12$	$0.770E-3$	$0.247E-3$

$x=0.5$	y_1	y_2	y_3
order 1 (2.11)	$0.371E-4$	$0.946E-8$	$0.210E-14$
order 2 (2.15)	$0.967E-8$	$0.104E-10$	$0.875E-26$
order 3 (2.21)	$0.251E-11$	$0.183E-11$	$0.868E-26$

$x=1$	y_1	y_2	y_3
order 1 (2.11)	$0.706E-4$	$0.898E-16$	$0.443E-29$
order 2 (2.15)	$0.184E-7$	$0.181E-21$	0
order 3 (2.21)	$0.479E-11$	$0.475E-22$	0

Problem 3

Absolute error

$(h=1/2^6)$

$x=0.0625$	y_1	y_2	y_3
order 1 (2.11)	$0.491D-5$	$0.055E+0$	$0.014D+0$
order 2 (2.15)	$0.127D-8$	$0.706D-2$	$0.552D-3$
order 3 (2.21)	$0.333D-12$	$0.770D-3$	$0.247D-3$

$x=0.5$	y_1	y_2	y_3
order 1 (2.11)	$0.411D-4$	$0.946D-8$	$0.210D-14$
order 2 (2.15)	$0.106D-7$	$0.104D-10$	$0.875D-26$
order 3 (2.21)	$0.278D-11$	$0.183D-11$	$0.868D-26$

$x=1$	y_1	y_2	y_3
order 1 (2.11)	$0.864D-4$	$0.898D-16$	$0.443D-29$
order 2 (2.15)	$0.224D-7$	$0.181D-21$	0.0
order 3 (2.21)	$0.585E-11$	$0.475D-22$	0.0

Finally we consider a variable step algorithm. Let y_n and $\tilde{y}_n$ denote the approximation to the i-th component at $x=x_n$ using step size h and $h/2$ respectively.

Defining

$$\begin{aligned} EST &= \| y_n - \tilde{y}_n \| \\ &= \max_i | y_n^{(i)} - \tilde{y}_n^{(i)} |, \end{aligned}$$

we use the following step size control policy for a given local accuracy requirement ε.

1. If $EST > \varepsilon$, reject the solution and half the step size h.
2. $\varepsilon > EST$, accept the solution and keep the step size h fixed.
3. $EST < \varepsilon/50$, accept the solution and double the step size h.

To test our automatic step control policy, we consider the problem (II) and (III) with $\varepsilon = 0.1E-4$. and the initial step size $h=1/16$.

Problem 2

	number of steps		Absolute error	
$x=0.00244...$		y_1	y_2	y_3
order 1 (2.11)	12	$0.588D-8$	$0.685D-3$	$0.050D-1$
order 2 (2.15)	12	$0.480E-13$	$0.449E-5$	$0.888E-4$
order 3 (2.21)	12	$0.138E-16$	$0.276E-7$	$0.120E-5$

$x=0.051...$		y_1	y_2	y_3
order 1 (2.11)	112	$0.122E-6$	$0.124E-2$	$0.282E-3$
order 2 (2.15)	112	$0.100E-11$	$0.821E-5$	$0.532E-5$
order 3 (2.21)	82	$0.971E-16$	$0.680E-6$	$0.765E-6$

$x=0.107...$		y_1	y_2	y_3
order 1 (2.11)	255	$0.255E-6$	$0.588E-3$	$0.687E-6$
order 2 (2.15)	226	$0.362E-11$	$0.214E-5$	$0.354E-7$
order 3 (2.21)	102	$0.167E-14$	$0.884E-6$	$0.410E-7$

Problem 3

	number of steps		Absolute error	
$x=0.0024...$		y_1	y_2	y_3
order 1 (2.11)	12	$0.603E-8$	$0.685E-3$	$0.050E-1$
order 2 (2.15)	12	$0.489E-13$	$0.449E-5$	$0.888E-4$
order 3 (2.21)	12	$0.227E-16$	$0.276E-7$	$0.120E-5$

$x=0.051...$		y_1	y_2	y_3
order 1 (2.11)	112	$0.127E-6$	$0.124E-2$	$0.282E-3$
order 2 (2.15)	107	$0.103E-11$	$0.821E-5$	$0.532E-5$
order 3 (2.21)	82	$0.194E-15$	$0.680E-6$	$0.765E-6$

$x=0.107...$		y_1	y_2	y_3
order 1 (2.11)	212	$0.249E-6$	$0.209E-3$	$0.147E-5$
order 2 (2.15)	197	$0.416E-11$	$0.185E-5$	$0.218E-7$
order 3 (2.21)	102	$0.185E-14$	$0.884E-6$	$0.410E-7$

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