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High order second derivative methods with Runge–Kutta stability for the numerical solution of stiff ODEs

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Abstract

We describe the construction of second derivative general linear methods (SGLMs) of orders five and six. We will aim for methods which are A–stable and have Runge–Kutta stability property. Some numerical results are given to show the efficiency of the constructed methods in solving stiff initial value problems.

Keywords: Ordinary differential equation; General linear methods; Runge–Kutta stability; A–stability; Second derivative methods.

1 Introduction

In many fields such as control theory, chemical kinetics, biology and the movement of stars in galaxies, dynamic behavior is modeled by systems of ordinary differential equations (ODEs). We consider the autonomous ODEs in the form

$$\begin{aligned} &y'(x) = f(y(x)), \qquad x \in [x_0, \overline{x}], \\ &y(x_0) = y_0, \end{aligned} \tag{1}$$

where $f : \mathbb{R}^m \to \mathbb{R}^m$ and m is the dimensionality of the system. We restrict our attention to autonomous systems because non-autonomous systems can be made autonomous by adding an extra equation to the system.

For system (1), let $g := f_y f$. For problems in which g can be calculated along with f, at a moderate additional cost, second derivative methods become feasible. General linear methods (GLMs) [6, 7, 12] as a unifying

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framework for the traditional methods, like Runge–Kutta methods, linear multistep methods, predictor–corrector methods and hybrid methods, have been extended to the second derivative general linear methods (SGLMs) by Butcher and Hojjati [8]. These methods which are s-stage and r-value, for the numerical solution of (1) are given by

$$\begin{aligned} Y^{[n]} &= h(A\otimes I_m)F(Y^{[n]}) + h^2(\overline{A}\otimes I_m)G(Y^{[n]}) + (U\otimes I_m)y^{[n-1]},\\ y^{[n]} &= h(B\otimes I_m)F(Y^{[n]}) + h^2(\overline{B}\otimes I_m)G(Y^{[n]}) + (V\otimes I_m)y^{[n-1]}, \end{aligned} \tag{2}$$

where h is the stepsize, A, $\overline{A}\in\mathbb{R}^{s\times s}$, $U\in\mathbb{R}^{s\times r}$, B, $\overline{B}\in\mathbb{R}^{r\times s}$ and $V\in\mathbb{R}^{r\times r}$ and notation $\otimes$ is the Kronecker product. Here, $Y^{[n]}=[Y_i^{[n]}]_{i=1}^s$ is an approximation of stage order q to the vector $y(x_{n-1}+ch)=[y(x_{n-1}+c_ih)]_{i=1}^s$, i.e.

$$Y_i^{[n]} = \sum_{k=0}^{q}\frac{c_i^k}{k!}h^k y^{(k)}(x_{n-1}) + O(h^{q+1}),\quad i=1,2,\ldots,s, \tag{3}$$

$F(Y^{[n]}):=[f(Y_i^{[n]})]_{i=1}^s$ and $G(Y^{[n]}):=[g(Y_i^{[n]})]_{i=1}^s$ where the vector $c=[c_1\ \ c_2\ \ \cdots\ \ c_s]^T$ is the abscissa vector. Also the vectors $y^{[n-1]}=[y_i^{[n-1]}]_{i=1}^r$ and $y^{[n]}=[y_i^{[n]}]_{i=1}^r$ are the input and output vectors at the step number n, respectively, which for a method of order p take the following forms

$$y_i^{[n-1]} = \sum_{k=0}^{p}\alpha_{ik}h^k y^{(k)}(x_{n-1}) + O(h^{p+1}),\quad i=1,2,\ldots,r, \tag{4}$$

and

$$y_i^{[n]} = \sum_{k=0}^{p}\alpha_{ik}h^k y^{(k)}(x_{n}) + O(h^{p+1}),\qquad i=1,2,\ldots,r, \tag{5}$$

for some $\alpha_{ik}\in\mathbb{R}$ associated with the method.

The main features of SGLMs including pre-consistency, consistency, zero-stability and types of these methods have been discussed in [3]. It has been shown in [4] that the SGLM (2) with the input vector (4) has order p and stage order $q=p$ iff

$$e^{cz} = zAe^{cz} + z^2\overline{A}e^{cz} + Uw(z) + O(z^{p+1}), \tag{6}$$

$$e^{z}w(z) = zBe^{cz} + z^2\overline{B}e^{cz} + Vw(z) + O(z^{p+1}). \tag{7}$$

where

$$e^{cz} = \left[e^{c_1z}\ \ e^{c_2z}\ \ \cdots\ \ e^{c_sz}\right]^T,$$

and $w(z)$ is a vector with elements given by

$$w_i(z) = \sum_{k=0}^{p}\alpha_{ik}z^k,\qquad i=1,2,\cdots,r.$$

In the special SGLMs with $p = q = r = s$, $U = I_s$ and $V\mathrm{e} = \mathrm{e}$, $\mathrm{e} = [1, 1, \ldots, 1]^T \in \mathbb{R}^s$, an equivalent condition for order conditions has been found in [5] as

$$B = B_0 - AB_1 - \overline{A}B_2 - VB_3 - (\overline{B} - V\overline{A})B_4 + VA,$$

where the (i, j) elements of B_0, B_1, B_2, B_3, and B_4 are given respectively by

$$\frac{\int_0^{1+c_i} \phi_j(x)dx}{\phi_j(c_j)}, \qquad \frac{\phi_j(1+c_i)}{\phi_j(c_j)}, \qquad \frac{\phi_j'(1+c_i)}{\phi_j(c_j)}, \qquad \frac{\int_0^{c_i} \phi_j(x)dx}{\phi_j(c_j)}, \qquad \frac{\phi_j'(c_i)}{\phi_j(c_j)}.$$

Here,

$$\phi_i(x) = \prod_{j=1, j\neq i}^{s} (x - c_j), \qquad i = 1, 2, \cdots, s.$$

Construction of SGLMs which are also suitable for the numerical solution of differential algebraic equations (DAEs) has been discussed in [10]. Some obtained order barries for different types of SGLMs, found in [3,4,10], are useful in construction of these methods. These barriers have been also confirmed by means of order arrows by Abdi and Butcher [1, 2]. Recently, efficiency of these methods in solving stiff ODEs arising from chemical reactions has been shown in [11].

In continuation of studying on SGLMs, in this paper we construct A–stable methods of orders five and six with $r = s = 3$ and Runge–Kutta stability property.

Next sections of this paper are organized as follows: In Sec. 2, we discuss about stability behaviour of Runge–Kutta stable three-stage methods. Sec. 3 is devoted to construction of SGLMs of orders five and six with A–stability property. Some numerical experiments are given in Sec. 4 to demonstrate the efficiency of the constructed methods.

2 RKS three-stage methods

We first recall that the stability matrix for SGLMs can be obtained by applying the methods to the standard test problem of Dahlquist [9] $y' = \zeta y$, where ζ is a complex number, which it is

$$M(z) = V + \left(zB + z^2\overline{B}\right)\left(I - zA - z^2\overline{A}\right)^{-1}U,$$

where $z = h\zeta$. Thus, we are interested in stable behavior of powers of $M(z)$. If $M(z)$ has only a single non-zero eigenvalue, $R(z)$, then the method is said to possess Runge-Kutta stability (RKS) property. For RKS methods, the stability behaviour is related to $R(z)$.
For the methods in which coefficient matrices A and $\overline{A}$ are lower triangular

with the same elements λ and μ on the diagonal, respectively, $R(z)$ takes the form

$$R(z) = \frac{N(z)}{(1-\lambda z - \mu z^2)^s}, \tag{8}$$

where $\deg(N) \leq 2s$. For the methods of order five and six with three stages that will be discussed in Sec. 3, the polynomial N defined in (8) satisfies

$$N(z) = (1-\lambda z - \mu z^2)^3 e^z - C_5 z^6 + O(z^7),$$

and

$$N(z) = (1-\lambda z - \mu z^2)^3 e^z + O(z^7),$$

respectively, for an arbitrary C_5 as the error constant of the method. For the method of order six, the error constant is

$$C_6 = \frac{1}{5040} - \frac{1}{240}\lambda - \frac{1}{40}\mu + \frac{1}{4}\lambda\mu + \big(\frac{1}{40} - \frac{1}{2}\mu\big)\lambda^2 + \big(\frac{1}{2} - \frac{3}{2}\lambda\big)\mu^2 - \frac{1}{24}\lambda^3 - \mu^3.$$

For these methods to be A–stable, using E-polynomial theorem [7], it is necessary and sufficient that $\lambda > 0$, $\mu < 0$, and so that the $E(y)$ is non-negative for y real where the E-polynomial is defined by

$$E(y) = |1 - \lambda \mathbf{i} y + \mu y^2|^6 - |N(\mathbf{i}y)|^2,$$

where $\mathbf{i}$ is the imaginary unit. The boundary of the regions of A-stable choices of (λ, μ) for the methods of order five (with different values of C_5) and order six are plotted in Figure 1 and Figure 2.

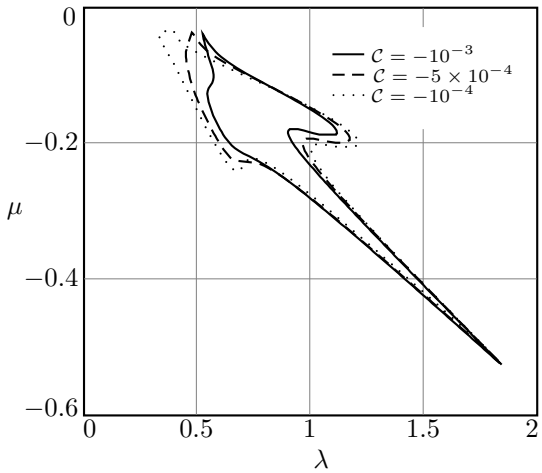

Figure 1: The boundary of the regions of A–stable choices of (λ, μ) for $s = 3$, $p = 5$ corresponding to $\mathcal{C} = -10^{-3}, -5 \times 10^{-4}, -10^{-4}$

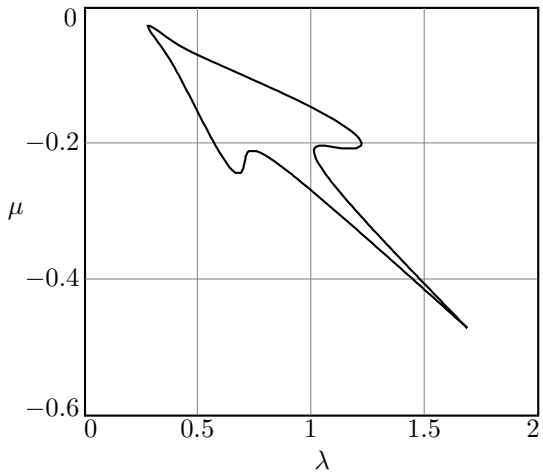

Figure 2: The boundary of the region of A–stable choices of (λ, μ) for $s = 3$, $p = 6$

3 *A*–stable RKS methods of orders 5 and 6

Construction SGLMs of orders $p = q \leq 4$ has been discussed in [3–5, 10]. In this section, we construct A–stable three-stage methods of orders five and six with RKS property. Throughout the construction of these methods, we will consider $U = I_s$ and $V = \mathrm{e}v^T$ where $v \in \mathbb{R}^r$ and $v^T\mathrm{e} = 1$. The later guarantees zero-stability of the methods [3].

3.1 Order 5 methods

Choosing $c = [0 \ \frac{1}{2} \ 1]^T$, $(\lambda, \mu) = (0.6, -0.1)$ from the intersection of the regions in Figure1 and solving the order conditions and the nonlinear RKS conditions, the coefficients matrices of the method take the following forms

$$A = \begin{bmatrix} 0.6000000000 & 0 & 0 \\ 0.4538633794 & 0.6000000000 & 0 \\ 0.8442059328 & 0.8999163314 & 0.6000000000 \end{bmatrix},$$

$$\overline{A} = \begin{bmatrix} -0.1000000000 & 0 & 0 \\ -0.1450566118 & -0.1000000000 & 0 \\ -0.9847293116 & -0.1278647721 & -0.1000000000 \end{bmatrix},$$

$$B = \begin{bmatrix} 0.3902646263 & 0.4639576064 & 0.2524239604 \\ -0.3312778090 & 1.1306242731 & 0.3534363496 \\ 5.0478598121 & -4.1644469839 & -0.5208888994 \end{bmatrix},$$

$$\overline{B} = \begin{bmatrix} -0.2677332867 & -0.3732899225 & -0.0223237563 \\ -0.4095181371 & -0.6362626571 & -0.0357186615 \\ 0.5750983052 & 1.6053219094 & 0.0622616286 \end{bmatrix},$$

$$v = \begin{bmatrix} 1.2203054517 & -0.3423946125 & 0.1220891608 \end{bmatrix}^T.$$

This method is A–stable with the error constant $C_5 \approx -3.50 \times 10^{-4}$.

3.2 Order 6 methods

Choosing $c = [0 \;\; c_1 \;\; 1]^T$, c_1 as a free parameter, and solving the order conditions and the nonlinear RKS conditions, we get $c_1 = -1.4989329045$ and the coefficients matrices of the method take the following forms

$$A = \begin{bmatrix} 0.4007120047 & 0 & 0 \\ 0.5574459850 & 0.4007120047 & 0 \\ 0.7281456081 & 0.0121320319 & 0.4007120047 \end{bmatrix},$$

$$\overline{A} = \begin{bmatrix} -0.0612701047 & 0 & 0 \\ -0.0145743957 & -0.0612701047 & 0 \\ 0.3881180321 & 0.1117302066 & -0.0612701047 \end{bmatrix},$$

$$B = \begin{bmatrix} 1.1371686053 & 0.2249968367 & 0.0903218055 \\ -0.0512895056 & 0.1078326109 & -0.6604347472 \\ 1.5642870990 & 0.3929237249 & -0.2450012162 \end{bmatrix},$$

$$\overline{B} = \begin{bmatrix} -0.0425486219 & 0.0078897842 & -0.0128566928 \\ 0.1945434509 & -0.0296649869 & 0.0449770864 \\ 0.3584398092 & 0.0701030286 & -0.0116769898 \end{bmatrix},$$

$$v = \begin{bmatrix} 0.8572479903 & 0.2113738061 & -0.0686217964 \end{bmatrix}^T.$$

The obtained value for (λ, μ) is the interior of the region of A–stable choices presented in Figure 2. The error constant for this A–stable method is $C_6 \approx 2.56 \times 10^{-5}$.

4 Numerical verifications

In this section we present some numerical results by applying the constructed methods of orders five and six in Sec. 3, in order to demonstrate the theoretical expectations. Computational experiments are carried out by applying the methods to the following two stiff problems.

S1– The non-linear stiff test problem

$$\begin{cases} y_1'(x) = -1002y_1(x) + 1000y_2^2(x),\ y_1(0) = 1, \\ y_2'(x) = y_1(x) - y_2(x)(1 + y_2(x)),\ y_2(0) = 1. \end{cases}$$

The exact solution is $y_1(x) = \exp(-2x)$ and $y_2(x) = \exp(-x)$ and $x \in [0, 1]$.

S2– The stiff initial value problem arose from a chemistry problem

$$\begin{cases} y_1'(x) = -0.013y_2 - 1000y_1y_2 - 2500y_1y_3,\ y_1(0) = 0, \\ y_2'(x) = -0.013y_2 - 1000y_1y_2, \qquad\qquad\quad y_2(0) = 1, \\ y_3'(x) = -2500y_1y_3, \qquad\qquad\qquad\quad y_3(0) = 1. \end{cases}$$

The reference solution at $x = 2$ is

$$\begin{aligned} y_1(2) &= -0.3616933169289 \times 10^{-5}, \\ y_2(2) &= 0.9815029948230, \\ y_3(2) &= 1.018493388244. \end{aligned}$$

Numerical results for the Problem S1, reported in Table 1, illustrate accuracy of the methods of order 5 and 6. These results are obtained with fixed stepsizes $h = 1/2^k$ with several integer values for k. In this table, we have listed norm of error $\|e_h(x)\|$ at the endpoint of integration $x = 1$. Also, in this table, the rows p refer to the numerical estimates to the order of

convergence, computed by the formula $p = \log_2(\|e_h(x)\|/\|e_{h/2}(x)\|)$ where $e_h(x)$ and $e_{h/2}(x)$ are errors corresponding to stepsizes h and $h/2$.

Table 1: The global error at the end of the interval of integration $[0, 1]$ for problem S1

h	2^{-2}	2^{-3}	2^{-4}	2^{-5}
Order 5 method	2.25×10^{-7}	5.61×10^{-9}	1.51×10^{-10}	4.34×10^{-12}
p		5.33	5.22	5.12
Order 6 method	6.92×10^{-8}	2.94×10^{-10}	2.45×10^{-12}	5.03×10^{-14}
p		7.88	6.91	5.61

Numerical results for the Problem S2 are given in Table 2 with stepsize $h = 0.001$. Comparing the obtained results by the methods with the reference solution shows the efficiency of the methods for solving stiff non-linear problems.

Table 2: Numerical results for problem S2 solved by the methods of orders five and six

x	y	Order 5 method	Order 6 method
	y_1	$-0.3616933169478728 \times 10^{-5}$	$-0.3616933215630078 \times 10^{-5}$
2	y_2	0.9815029948594308	0.9815030036954803
	y_3	1.018493388207507	1.018493379371295

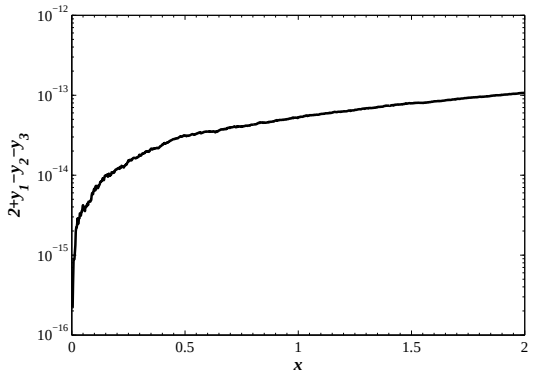

Figure 3: Variation of $2 + y_1 - y_2 - y_3$ versus x which y_1, y_2 and y_3 are the numerical solutions obtained by the method of order 5

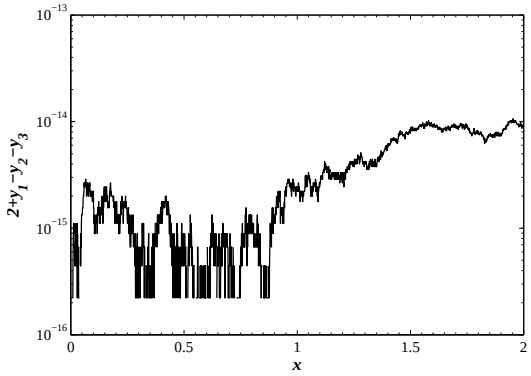

Figure 4: Variation of $2 + y_1 - y_2 - y_3$ versus x which y_1, y_2 and y_3 are the numerical solutions obtained by the method of order 6

The differential equations in Problem S2 satisfy a linear conservation law

$$2 + y_1(x) - y_2(x) - y_3(x) = 0, \tag{9}$$

for all x. In Figure 3 and Figure 4, we have plotted the graph of $2+y_1-y_2-y_3$ versus x. We observe that for both methods of orders five and six equation (9) for the obtained numerical solutions holds approximately with high accuracy which demonstrate the accuracy of the applied methods.

5 Conclusion

For methods of higher orders ($p \geq 5$) with $p = q = r = s$, it is no longer possible to solve the nonlinear systems of equations for satisfying RKS property by symbolic manipulation packages [5]. It seems that this difficulty does not appear for methods with fewer stages. In this paper we constructed RKS methods of orders $p = 5$ and $p = 6$ with $r = s = 3$.

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روش‌های مشتق دوم مرتبه بالا با پایداری رانگ-کوتا برای حل عددی معادلات دیفرانسیل معمولی سخت

علی عبدی و غلامرضا حجتی

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چکیده : ساخت روش-های خطی عمومی مشتق دوم (SGLMs) از مراتب پنج و شش را بحث و توصیف می کنیم. در این بررسی، روش-های ساخته شده A - پایدار بوده و دارای خاصیت پایداری رانگ-کوتا هستند. برخی نتایج عددی برای نشان دادن کارایی روش-های ساخته شده برای حل مسائل مقدار اولیه سخت ارائه می شوند .

کلمات کلیدی : معادله دیفرانسیل معمولی؛ روش-های خطی عمومی؛ پایداری رانگ-کوتا؛ A - پایداری؛ روش-های مشتق دوم.