

Highly stable general linear methods for differential systems

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Abstract. We describe search for A -stable and algebraically stable general linear methods of order p and stage order $q = p$ or $q = p - 1$. The search for A -stable methods is based on the Schur criterion applied for specific methods with stability polynomial of reduced degree. The search for algebraically stable methods is based on the sufficient conditions proposed recently by Hill.

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1. INTRODUCTION

We describe the search for highly stable general linear methods (GLMs) for ordinary differential equations (ODEs)

$$\begin{cases} y'(t) = f(y(t)), & t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \quad (1.1)$$

where the function $f: \mathbf{R}^m \rightarrow \mathbf{R}^m$ is assumed to be sufficiently smooth and $y_0 \in \mathbf{R}^m$ is a given initial value. Let N be a positive integer and define the grid $t_n = t_0 + nh$, $n = 0, 1, \dots, N$, $Nh = T - t_0$. GLMs for the numerical solution of (1.1) are defined by

$$\begin{cases} Y_i^{[n]} = h \sum_{j=1}^s a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^r u_{ij} z_j^{[n-1]}, & i = 1, 2, \dots, s, \\ z_i^{[n]} = h \sum_{j=1}^s b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^r v_{ij} z_j^{[n-1]}, & i = 1, 2, \dots, r, \end{cases} \quad (1.2)$$

$n = 1, 2, \dots, N$. Here, the internal stages $Y_i^{[n]}$ are approximations of stage order q to $y(t_{n-1} + c_i h)$ and the external stages $z_i^{[n]}$ are approximations of order p to the linear combinations of scaled derivatives of $y(t_n)$, compare [4], [12]. These methods are specified by the abscissa vector $\mathbf{c} = [c_1, \dots, c_s]^T$ and four coefficient matrices $\mathbf{A} = [a_{ij}]$, $\mathbf{U} = [u_{ij}]$, $\mathbf{B} = [b_{ij}]$, and $\mathbf{V} = [v_{ij}]$.

In Section 2 we review the concepts of A - and algebraic stability and in Section 3 we describe tools to search for methods with appropriate stability properties. The paper concludes with examples of A - and algebraically stable methods given in Section 4.

2. STABILITY CONCEPTS

Applying the GLM (1.2) to the linear test equation $y' = \xi y$, $t \geq 0$, $\xi \in \mathbb{C}$, we obtain the recurrence relation $z^{[n]} = \mathbf{S}(z) z^{[n-1]}$, $n = 1, 2, \dots$, $z = h\xi$. Here, $\mathbf{S}(z)$ is the stability matrix defined by $\mathbf{S}(z) = \mathbf{V} + z\mathbf{B}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{U}$. We also define the stability function $p(\eta, z) = \det(\eta\mathbf{I} - \mathbf{S}(z))$. Denote by $\eta_1(z), \eta_2(z), \dots, \eta_r(z)$ the roots of the stability function $p(\eta, z)$. Then the region of absolute stability of GLM (1.2) is given by

$$\mathcal{A} = \left\{ z \in \mathbb{C} : |\eta_i(z)| < 1, i = 1, 2, \dots, r \right\}.$$

The GLM (1.2) is said to be A -stable if its region of absolute stability includes the negative complex plane $\mathbb{C}^- = \{z \in \mathbb{C} : \operatorname{Re}(z) < 0\}$, i.e., $\mathbb{C}^- \subset \mathcal{A}$.

We are also interested in algebraic stability. The GLM (1.2) is said to be algebraically stable, if there exist a real, symmetric and positive definite matrix $\mathbf{G} \in \mathbf{R}^{r \times r}$ and a real, diagonal and positive definite matrix $\mathbf{D} \in \mathbf{R}^{s \times s}$ such that the matrix $\mathbf{M} \in \mathbf{R}^{(s+r) \times (s+r)}$ defined by

$$\mathbf{M} = \left[\begin{array}{c|c} \mathbf{DA} + \mathbf{A}^T \mathbf{D} - \mathbf{B}^T \mathbf{GB} & \mathbf{DU} - \mathbf{B}^T \mathbf{GV} \\ \hline \mathbf{U}^T \mathbf{D} - \mathbf{V}^T \mathbf{GB} & \mathbf{G} - \mathbf{V}^T \mathbf{GV} \end{array} \right] \quad (2.1)$$

is nonnegative definite. The significance of this definition follows from the result proved by Butcher [2], [3] (see also [1], [9]), that for a preconsistent and non-confluent GLMs (1.2), i.e., methods with distinct abscissas c_i , $i = 1, 2, \dots, s$, algebraic stability is equivalent to G -stability. This last concept is related to the test equation

$$y'(t) = g(t, y(t)), \quad t \geq 0, \quad (2.2)$$

where g satisfies the one-sided Lipschitz condition of the form $(g(t, y_1) - g(t, y_2))^T (y_1 - y_2) \leq 0$ for all $t \geq 0$ and $y_1, y_2 \in \mathbf{R}^m$. Denote by $y(t)$ and $\tilde{y}(t)$ two solutions to (2.2) with initial conditions y_0 and \tilde{y}_0 , respectively. Then it is known that

$$\|y(t_2) - \tilde{y}(t_2)\| \leq \|y(t_1) - \tilde{y}(t_1)\| \quad (2.3)$$

for $0 \leq t_1 \leq t_2$, compare [8], [5]. Here, $\|\cdot\|$ is any norm in \mathbf{R}^m . The method (1.2) is said to be G -stable if it inherits the property (2.3), i.e.,

$$\|z^{[n+1]} - \tilde{z}^{[n+1]}\|_G \leq \|z^{[n]} - \tilde{z}^{[n]}\|_G, \quad (2.4)$$

for all step sizes $h > 0$ and for all differential systems (2.2) with the function g satisfying the one-sided Lipschitz condition. Here, $z^{[n]}$ and $\tilde{z}^{[n]}$ are solutions to (1.2) obtained with initial vectors $z^{[0]}$ and $\tilde{z}^{[0]}$, and $\|\cdot\|_G$ is the norm generated by the matrix \mathbf{G} . For the vector $y \in \mathbf{R}^{mr}$ composed of the subvectors $y_i \in \mathbf{R}^m$, $i = 1, 2, \dots, r$, this norm is defined by

$$\|y\|_G^2 = \sum_{i=1}^r \sum_{j=1}^r g_{ij} y_i^T y_j.$$

3. TOOLS TO INVESTIGATE STABILITY

It can be verified that the stability function $p(\eta, z)$ of the method (1.2) takes the form

$$p(\eta, z) = \eta^{r+1} - R_1(z)\eta^r + R_2(z)\eta^{r-1} + \dots + (-1)^r R_r(z)\eta + (-1)^{r+1} R_{r+1}(z), \quad (3.1)$$

where $R_i(z)$ are rational functions

$$R_i(z) = \frac{p_i(z)}{p_0(z)}, \quad i = 1, 2, \dots, r,$$

with

$$\begin{aligned} p_0(z) &= 1 + p_{01}z + \dots + p_{0s}z^s, & p_1(z) &= 1 + p_{11}z + \dots + p_{1s}z^s, \\ p_2(z) &= p_{21}z + \dots + p_{2s}z^s, \dots, & p_s(z) &= p_{s,s-1}z^{s-1} + p_{ss}z^s, & p_{s+1}(z) &= p_{s+1,s}z^s. \end{aligned}$$

To investigate stability properties of GLMs (1.2) it is more convenient to work with the polynomial

$$\tilde{p}(\eta, z) = p_0(z)p(\eta, z) \quad (3.2)$$

instead of the rational function $p(\eta, z)$ and we will always adopt this approach. The GLM (1.2) is A -stable if $\tilde{p}(\eta, z)$ is a Schur polynomial, i.e., if the roots $\eta_i(z)$, $i = 1, 2, \dots, s+1$, of $\tilde{p}(\eta, z)$ are in the unit circle for all z such that $\text{Re}(z) < 0$. It follows from the maximum principle that this is the case if the roots of $p_0(z)$ are in the positive half plane $\mathbb{C}^+ = \{z : \text{Re}(z) > 0\}$ and $\tilde{p}(\eta, iy)$ is a Schur polynomial for $y \in \mathbf{R}$. This last condition can be investigated using Schur criterion [15] as explained in [12].

Search for algebraically stable methods can be done numerically, using the criterion for algebraic stability which is based on the Nyquist stability function defined by

$$\mathbf{N}(\xi) = \mathbf{A} + \mathbf{U}(\xi\mathbf{I} - \mathbf{V})^{-1}\mathbf{B}, \quad \xi \in \mathbb{C} - \sigma(\mathbf{V}). \quad (3.3)$$

Here, $\sigma(\mathbf{V})$ stands for the spectrum of the matrix \mathbf{V} . This terminology of the Nyquist stability function was suggested by Hill [11], although this function in the context of GLMs was first introduced by Butcher [3], who did not assign to it any specific name. Denote by $\tilde{\mathbf{w}}$ a principal left eigenvector of \mathbf{V} , i.e., the vector such that $\tilde{\mathbf{w}}^T \mathbf{V} = \tilde{\mathbf{w}}^T$, $\tilde{\mathbf{w}}^T \mathbf{q}_0 = 1$, where \mathbf{q}_0 is the preconsistency vector of GLM (2.2). Following [11] define the diagonal matrix $\tilde{\mathbf{D}}$ by $\tilde{\mathbf{D}} = \text{diag}(\mathbf{B}^T \tilde{\mathbf{w}})$, and following [3], define by $\text{He}(\mathbf{Q})$ the Hermitian part of a complex square matrix \mathbf{Q} , i.e., $\text{He}(\mathbf{Q}) = (\mathbf{Q} + \mathbf{Q}^*)/2$, where \mathbf{Q}^* stands for the conjugate transpose of \mathbf{Q} . Then it was demonstrated in [3] and [11] that a consistent GLM (2.2) is algebraically stable if the following conditions are satisfied:

1. The coefficient matrix \mathbf{V} is power-bounded.
2. $\mathbf{U}\mathbf{x} \neq \mathbf{0}$ for all right eigenvectors of \mathbf{V} and $\mathbf{B}^T \mathbf{x} \neq \mathbf{0}$ for all left eigenvectors of \mathbf{V} .
3. $\tilde{\mathbf{D}} > 0$ and $\text{He}(\tilde{\mathbf{D}}\mathbf{A}) \geq 0$.
4. $\text{He}(\tilde{\mathbf{D}}\mathbf{N}(\xi)) \geq 0$ for all ξ such that $|\xi| = 1$ and $\xi \in \mathbb{C} - \sigma(\mathbf{V})$.

4. EXAMPLES OF A- AND ALGEBRAICALLY STABLE METHODS

In this section we will illustrate the search for A- and algebraically stable methods for the class of two-step Runge-Kutta methods defined by

$$\begin{cases} Y_i^{[n]} = y_{n-1} + h \sum_{j=1}^s (a_{ij} f(Y_j^{[n]}) + b_{ij} f(Y_j^{[n-1]})), & i = 1, 2, \dots, s, \\ y_n = y_{n-1} + h \sum_{j=1}^s (v_j f(Y_j^{[n]}) + w_j f(Y_j^{[n-1]})), \end{cases} \quad (4.1)$$

$n = 1, 2, \dots, N$. Here, y_n is an approximation to $y(t_n)$ and $Y_i^{[n]}$ are approximations to $y(t_{n-1} + c_i h)$, $i = 1, 2, \dots, s$, where $y(t)$ is the solution to (1.1). These methods were introduced by Jackiewicz and Tracogna [13] and further investigated in [14], [6], [10], [7]. We also refer to a recent monograph on general linear methods [12] where these formulas are discussed in chapters 5 and 6.

Putting $z^{[n]} = [y_n^T, h f(Y^{[n]})^T]^T$ the TSRK method (4.1) can be represented as GLM (1.2) with coefficient matrices \mathbf{A} , \mathbf{U} , \mathbf{B} and \mathbf{V} defined by

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{c|cc} A & e & B \\ v^T & 1 & w^T \\ I & 0 & 0 \end{array} \right]. \quad (4.2)$$

Solving the appropriate stage order and order conditions we obtain an eleven-parameter family of methods of order $p = 4$ and stage order $q = 4$ depending on $c_1, c_2, c_3, a_{ij}, i = 1, 2, 3, j = 1, 2, v_3$, and w_3 . Searching for A-stable methods we assume that the abscissa vector $c = [0, 1/2, 1]^T$. The stability polynomial (3.2) for this family of methods takes the form

$$\tilde{p}(\eta, z) = \eta (p_0(z)\eta^4 - p_1(z)\eta^3 + p_2(z)\eta^2 - p_3(z)\eta + p_4(z)).$$

where $p_i(z)$ are polynomials of degree 3 with respect to z . We compute next the parameters a_{11}, a_{12} , and a_{13} to annihilate polynomials $p_3(z)$ and $p_4(z)$. This leads to a five-parameter family of methods depending on $a_{22}, a_{31}, a_{32}, v_3$, and w_3 whose stability properties are determined by quadratic polynomial $p_0(z)\eta^2 - p_1(z)\eta + p_0(z)$. The results of computer search based on the Schur criterion are presented in Fig. 1 in the parameter space (v_3, w_3) for selected values of the parameters a_{22}, a_{31}, a_{32} .

We also searched for methods which are algebraically stable with general abscissa vector c . We have found formulas for which

$$\text{He}(\tilde{\mathbf{D}}\mathbf{N}(\xi)) \Big|_{\xi=e^{it}} \geq -3.50 \cdot 10^{-11}, \quad (4.3)$$

$t \in [0, 2\pi]$. This bound was obtained by dividing the interval $[0, 2\pi]$ into $n = 10000$ subintervals. Dividing $[0, 2\pi]$ into $n = 1000$ and $n = 100$ subintervals, these bounds are equal to 0. The coefficients of a method satisfying (4.3) are

$$c = [0.748023646320140 \quad -0.088623514454709 \quad 1.356515696201252]^T,$$

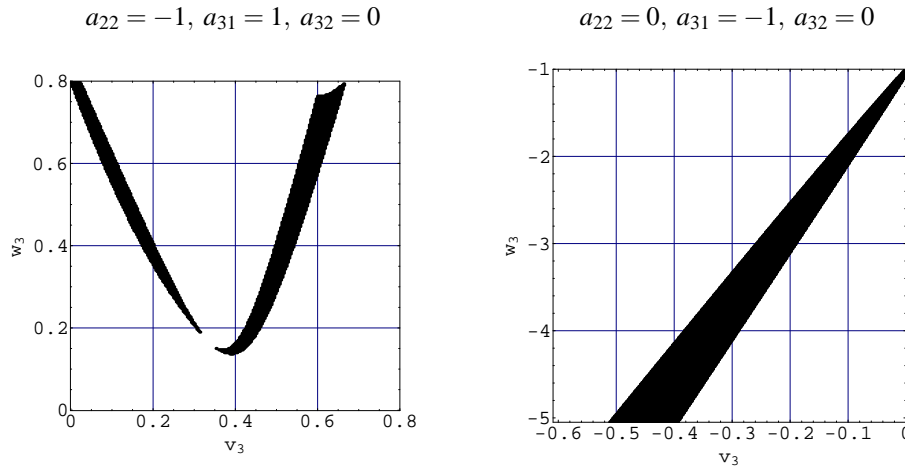


FIGURE 1. Regions of A -stability in the (v_3, w_3) -plane, for TSRK methods with $s = 3$ and $p = q = 4$, for specific values of the parameters a_{22} , a_{31} , a_{32} .

$$A = \begin{bmatrix} 0.421393024773032 & 0.363279074448260 & -0.048601648229138 \\ -0.136821530809582 & 0.352101387625363 & 0.033470857866822 \\ 0.730130053789655 & 0.254440972752177 & 0.213275751785994 \end{bmatrix},$$

$$B = \begin{bmatrix} -0.061994904923431 & -0.014321664726926 & 0.088269764978343 \\ -0.413117314149065 & 0.027004921378105 & 0.048738163633648 \\ -0.090220513163391 & 0.002986566608366 & 0.245902864428450 \end{bmatrix},$$

$$v = [0.622394316996030 \quad 0.313242750536090 \quad -0.011784503142076]^T,$$

$$w = [-0.062831671181596 \quad -0.008857653267082 \quad 0.147836760058631]^T.$$

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