Search for highly stable two-step Runge-Kutta methods

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by DMA "R.Caccioppoli" - Università di Napoli "Federico II" and by DMI - Università di Salerno.
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Abstract

We describe the search for A-stable and algebraically stable two-step Runge Kutta 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 criteria proposed recently by Hewitt and Hill.

Keywords: Two-step Runge-Kutta methods, order conditions, linear stability analysis, A-stability, algebraic stability.

1. Introduction

It is the purpose of this paper to describe our search for highly stable two-step Runge-Kutta (TSRK) methods for the numerical solution of the initial-value problem for ordinary differential equations (ODEs). We consider this initial-value problem in autonomous form

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

where the function $f : \mathbb{R}^m \to \mathbb{R}^m$ is assumed to be sufficiently smooth and $y_0 \in \mathbb{R}^m$ is a given initial value.

For the numerical solution of (1.1) we consider the general class of TSRK methods which on the uniform grid $t_n = t_0 + nh$, $n = 0, 1, \ldots, N$, $Nh = T - t_0$, are defined by the formulas

$$\begin{cases} Y_i^{[n]} = (1 - u_i)y_{n-1} + u_i y_{n-2} + h \displaystyle\sum_{j=1}^{s} \Big(a_{ij} f(Y_j^{[n]}) + b_{ij} f(Y_j^{[n-1]})\Big), \\ y_n = (1 - \vartheta)y_{n-1} + \vartheta y_{n-2} + h \displaystyle\sum_{j=1}^{s} \Big(v_j f(Y_j^{[n]}) + w_j f(Y_j^{[n-1]})\Big), \end{cases} \tag{1.2}$$

$n = 1, 2, \ldots, N$. Here, y_n is an approximation to $y(t_n)$ and $Y_i^{[n]}$ are approximations to $y(t_{n-1} + c_i h)$, $i = 1, 2, \ldots, s$, where $y(t)$ is the solution to (1.1). These methods were introduced by Jackiewicz and Tracogna [20] and further investigated in [21], [7], [15], [22], [8], [10]. We also refer to a recent monograph on general linear methods [19] where these formulas are discussed in chapters 5 and 6.

The TSRK methods (1.2) can be represented by the abscissa vector $c = [c_1, \ldots, c_s]^T$ and the following table of its coefficients

$$\begin{array}{c|c|c} u & A & B \\ \hline \vartheta & v^T & w^T \end{array} = \begin{array}{c|ccc|ccc} u_1 & a_{11} & \cdots & a_{1s} & b_{11} & \cdots & b_{1s} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ u_s & a_{s1} & \cdots & a_{ss} & b_{s1} & \cdots & b_{ss} \\ \hline \vartheta & v_1 & \cdots & v_s & w_1 & \cdots & w_s \end{array}.$$

In the last few years these methods were usually investigated under the assumption that the coefficient matrix A has the form

$$A = \begin{bmatrix} \lambda & & & \\ a_{21} & \lambda & & \\ \vdots & \ddots & \ddots & \\ a_{s1} & \cdots & a_{s,s-1} & \lambda \end{bmatrix},$$

$\lambda \geq 0$, where the explicit methods corresponding to $\lambda = 0$ are called type 1 methods and the implicit formulas corresponding to $\lambda > 0$ are called type 2 methods. Type 3 and type 4 methods for which A has the form

$$A = \operatorname{diag}(\lambda, \lambda, \ldots, \lambda),$$

with $\lambda = 0$ and $\lambda > 0$, respectively, were also investigated in [20], [19]. These restrictions on the matrix A were relaxed in [9], [19], where it was assumed that this matrix has a one point spectrum $\sigma(A) = \{\lambda\}$. In this paper we search for highly stable TSRK methods (1.2) without imposing any restrictions on the structure of the coefficient matrix A.

In this paper we only examine methods of order p and stage order $q = p$ or $q = p - 1$. Define the vectors

$$C_k = \frac{c^k}{k!} - \frac{(-1)^k}{k!}u - \frac{Ac^{k-1}}{(k-1)!} - \frac{B(c-e)^{k-1}}{(k-1)!},$$

$k = 1, 2, \ldots$, and the constants

$$\widehat{C}_k = \frac{1}{k!} - \frac{(-1)^k}{k!}\vartheta - \frac{v^T c^{k-1}}{(k-1)!} - \frac{w^T (c-e)^{k-1}}{(k-1)!},$$

$k = 1, 2, \ldots$, where $e = [1, \ldots, 1] \in \mathbb{R}^s$, and c^k denotes componentwise exponentiation. Then it was proved in [9], [19] that the method (1.2) has order p and stage order $q = p$ if and only if

$$C_k = 0, \quad \widehat{C}_k = 0, \quad k = 1, 2, \ldots, p. \tag{1.3}$$

Similarly, the methods (1.2) has order p and stage order $q = p - 1$ if and only if

$$C_k = 0, \quad k = 1, 2, \ldots, p, \quad \widehat{C}_k = 0, \quad k = 1, 2, \ldots, p-1. \tag{1.4}$$

In Section 2 we review various stability concepts in the context of general linear methods (GLMs) which includes TSRK methods (1.2) as special cases. In Section 3 we investigate TSRK methods (1.2) for which $\vartheta = 0$ and $u = 0$ and in Section 4 the general case with $\theta \neq 0$ and $u \neq 0$. In both cases, these methods are first reformulated as GLMs. The explicit expressions for the Nyquist stability functions $\mathbf{N}(\xi)$ and Hermitian parts of $\widetilde{\mathbf{D}}\mathbf{N}(\xi)$ are obtained in terms of the coeffcients of TSRK methods and the limits of $\widetilde{\mathbf{D}}\mathbf{N}(\xi)$ are computed as $\xi \to 1$ on the unit circle. These expression aid the derivation of highly stable TSRK methods. This is carried out in in Section 5 and 6, where we use the stability theory of GLMs reviewed in Section 2 to search for methods which are A-stable and algebraically stable. Examples of such methods with $\vartheta = 0$ and $u = 0$ and $\theta \neq 0$ and $u \neq 0$ up to order $p = 4$ and stage order $q = 4$ are given in Section 5 and Section 6, respectively. In Section 7 we review the example of algebraically stable method derived by Hewitt and Hill [16]. Finally, in Section 8 some concluding remarks are given and plans for future research are briefly outlined.

2. Stability concepts for general linear methods

It is well known that TSRK methods (1.2) form a subclass of GLMs for the numerical solution of ODEs (1.1). This very general class of methods is defined by

$$\begin{cases} Y_i^{[n]} = h\sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} z_j^{[n-1]}, & i = 1,2,\ldots,s, \\ z_i^{[n]} = h\sum_{j=1}^{s} b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} z_j^{[n-1]}, & i = 1,2,\ldots,r, \end{cases} \tag{2.1}$$

$n = 1,2,\ldots,N$. Here, the internal stages $Y_i^{[n]}$ are approximations of stage order q to $y(t_{n-1} + c_i h)$, i.e.,

$$Y_i^{[n]} = y(t_{n-1} + c_i h) + O(h^{q+1}),$$

and the external stages $z_i^{[n]}$ are approximations of order p to the linear combinations of scaled derivatives of $y(t_n)$, i.e.,

$$z_i^{[n]} = \sum_{k=0}^{p} q_{ik} h^k y^{(k)}(t_n) + O(h^{p+1}),$$

compare [19]. Putting

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix}, \quad hf(Y^{[n]}) = \begin{bmatrix} hf(Y_1^{[n]}) \\ \vdots \\ hf(Y_s^{[n]}) \end{bmatrix}, \quad z^{[n]} = \begin{bmatrix} z_1^{[n]} \\ \vdots \\ z_r^{[n]} \end{bmatrix},$$

the GLM (2.1) can be written in vector form as follows

$$\left[\begin{array}{c} Y^{[n]} \\ \hline z^{[n]} \end{array}\right] = \left[\begin{array}{c|c} \mathbf{A}\otimes\mathbf{I} & \mathbf{U}\otimes\mathbf{I} \\ \hline \mathbf{B}\otimes\mathbf{I} & \mathbf{V}\otimes\mathbf{I} \end{array}\right] \left[\begin{array}{c} hf(Y^{[n]}) \\ \hline z^{[n-1]} \end{array}\right], \tag{2.2}$$

$n = 1,2,\ldots,N$. Here, $\mathbf{I}$ is the identity matrix of dimension m and '$\otimes$' stands for Knonecker product of matrices. The connection between the order conditions of the TSRK method (1.2) and its representation as GLM is described in chapter 5 of [19]. The method (2.2) is zero-stable if the coefficient matrix $\mathbf{V}$ is power bounded. In the case of TSRK methods (1.2) this is equivalent to the condition

$$-1 < \vartheta \leq 1, \tag{2.3}$$

compare [19], [20].

Applying the GLM (2.2) to the linear test equation

$$y' = \xi y, \quad t \geq 0, \tag{2.4}$$

$\xi \in \mathbb{C}$, we obtain the recurrence relation

$$z^{[n]} = \mathbf{S}(z) z^{[n-1]},$$

$n = 1,2,\ldots$, $z = h\xi$. Here, $\mathbf{S}(z)$ is the stability matrix defined by

$$\mathbf{S}(z) = \mathbf{V} + z\mathbf{B}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{U}. \tag{2.5}$$

We also define the stability function

$$p(\eta, z) = \det(\eta\mathbf{I} - \mathbf{S}(z)). \tag{2.6}$$

Denote by $\eta_1(z), \eta_2(z), \ldots, \eta_r(z)$ the roots of the stability function $p(\eta, z)$. Then the region of absolute stability of GLM (2.2) is given by

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

The GLM (2.2) 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 review next the concepts of G-stability and algebraic stability for GLMs. Consider the initial-value problem

$$\begin{cases} y'(t) = g(t, y(t)), & t \geq 0, \\ y(0) = y_0, \end{cases} \tag{2.7}$$

$g : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$, where the function g satisfies the one-sided Lipschitz condition of the form

$$\left(g(t, y_1) - g(t, y_2)\right)^T (y_1 - y_2) \leq 0 \tag{2.8}$$

for all $t \geq 0$ and $y_1, y_2 \in \mathbb{R}^m$. Denote by $y(t)$ and $\widetilde{y}(t)$ two solutions to (2.7) with initial conditions y_0 and $\widetilde{y}_0$, respectively. Then it is known that the condition (2.8) implies that

$$\left\| y(t_2) - \widetilde{y}(t_2) \right\| \leq \left\| y(t_1) - \widetilde{y}(t_1) \right\| \tag{2.9}$$

for $0 \leq t_1 \leq t_2$, compare [11], [6]. Here, $\| \cdot \|$ is any norm in $\mathbb{R}^m$. The differential systems (2.7) with this property are called dissipative.

Let $\mathbf{G} = [g_{ij}]_{i,j=1}^r$ be a real, symmetric and positive definite matrix, and for a vector $y \in \mathbb{R}^{mr}$

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_r \end{bmatrix}, \quad y_i \in \mathbb{R}^m, \quad i = 1, 2, \ldots, r,$$

define the inner product norm $\| \cdot \|_G$ by

$$\|y\|_G^2 = \sum_{i=1}^r \sum_{j=1}^r g_{ij} y_i^T y_j. \tag{2.10}$$

Denote by $\{z^{[n]}\}_{n=0}^N$ the solution to (2.2) with initial value $z^{[0]}$, and by $\{\widetilde{z}^{[n]}\}_{n=0}^N$ the solution obtained by perturbing (2.2) or by using a different initial value $\widetilde{z}^{[0]}$. A numerical method which inherits the dissipativity property (2.9) of the solution $y(t)$ to (2.7) in the norm (2.10) is said to be G-stable. To be more precise, the GLM (2.2) is G-stable if there exists a real, symmetric and positive definite matrix $\mathbf{G} \in \mathbb{R}^{r \times r}$ such that for two numerical solutions $\{z^{[n]}\}_{n=0}^N$ and $\{\widetilde{z}^{[n]}\}_{n=0}^N$ we have

$$\left\| z^{[n+1]} - \widetilde{z}^{[n+1]} \right\|_G \leq \left\| z^{[n]} - \widetilde{z}^{[n]} \right\|_G, \tag{2.11}$$

for all step sizes $h > 0$ and for all differential systems (2.7) with the function g satisfying (2.8).

We next define algebraic stability. The GLM (2.2) is said to be algebraically stable, if there exist a real, symmetric and positive definite matrix $\mathbf{G} \in \mathbb{R}^{r \times r}$ and a real, diagonal and positive definite matrix $\mathbf{D} \in \mathbb{R}^{s \times s}$ such that the matrix $\mathbf{M} \in \mathbb{R}^{(s+r) \times (s+r)}$ defined by

$$\mathbf{M} = \left[\begin{array}{c|c} \mathbf{DA} + \mathbf{A}^T\mathbf{D} - \mathbf{B}^T\mathbf{GB} & \mathbf{DU} - \mathbf{B}^T\mathbf{GV} \\ \hline \mathbf{U}^T\mathbf{D} - \mathbf{V}^T\mathbf{GB} & \mathbf{G} - \mathbf{V}^T\mathbf{GV} \end{array} \right] \tag{2.12}$$

is nonnegative definite. The significance of this definition follows from the result proved by Butcher [3], [4] (see also [14]), that for a preconsistent and non-confluent GLMs (2.2), i.e., methods with distinct abscissas c_i, $i = 1, 2, \ldots, s$, algebraic stability is equivalent to G-stability.

In general, it is quite difficult to verify if a given GLM is algebraically stable, and even more difficult to construct new classes of GLMs which are algebraically stable. In our search for such methods we will use the fact, proved in [2], that for a preconsistent and algebraically stable GLM (2.2) the matrices $\mathbf{G}$ and $\mathbf{D}$ are not independent but related by the equation

$$\mathbf{D} = \operatorname{diag}(\mathbf{B}^T\mathbf{G}\mathbf{q}_0), \tag{2.13}$$

where $\mathbf{q}_0$ is the preconsistency vector, i.e., a vector satisfying the relations

$$\mathbf{U}\mathbf{q}_0 = \mathbf{e}, \quad \mathbf{V}\mathbf{q}_0 = \mathbf{q}_0,$$

and $\mathbf{e} = [1, \dots, 1]^T \in \mathbb{R}^s$, compare [19]. Moreover, $\mathbf{G}\mathbf{q}_0$ is a left eigenvector of the coefficient matrix $\mathbf{V}$ corresponding to the eigenvalue equal to one, i.e.,

$$(\mathbf{I} - \mathbf{V}^T)\mathbf{G}\mathbf{q}_0 = 0, \tag{2.14}$$

compare part ii) of Lemma 9.5 in [14].

We will write $\mathbf{M} \geq 0$ if the matrix $\mathbf{M}$ is nonnegative definite. It was observed by Hewitt and Hill [16], [17] that the verification if the matrix $\mathbf{M}$ is nonnegative definite can be simplified by the use of the result proved by Albert [1]. This result states that the matrix $\mathbf{M}$ given by

$$\mathbf{M} = \left[\begin{array}{c|c} \mathbf{M}_{11} & \mathbf{M}_{12} \\ \hline \mathbf{M}_{12}^T & \mathbf{M}_{22} \end{array}\right]$$

satisfies $\mathbf{M} \geq 0$ if and only if

$$\mathbf{M}_{11} \geq 0, \quad \mathbf{M}_{22} - \mathbf{M}_{12}^T\mathbf{M}_{11}^+\mathbf{M}_{12} \geq 0, \quad \mathbf{M}_{11}\mathbf{M}_{11}^+\mathbf{M}_{12} = \mathbf{M}_{12}, \tag{2.15}$$

or equivalently

$$\mathbf{M}_{22} \geq 0, \quad \mathbf{M}_{11} - \mathbf{M}_{12}\mathbf{M}_{22}^+\mathbf{M}_{12}^T \geq 0, \quad \mathbf{M}_{22}\mathbf{M}_{22}^+\mathbf{M}_{12}^T = \mathbf{M}_{12}^T \tag{2.16}$$

(see [16]). Here, $\mathbf{A}^+$ stands for the Moore-Penrose pseudoinverse of the matrix $\mathbf{A}$. We refer to [12] or [13] for the definition of this notion.

Although the criteria based on Albert theorem can be used to verify if specific examples of GLMs are algebraically stable, these criteria are not very practical to search for algebraically stable GLMs which depend on some number of unknown parameters. In such searches it is necessary to examine many inequalities which depend on the unknown coefficients of the matrix $\mathbf{G}$ and the remaining free parameters of GLMs and this task often exceeds the capabilities of symbolic manipulation packages such as Mathematica or Maple. However, there is a more practical approach, where this search can be done numerically, using the criterion for algebraic stability based on the Nyquist stability function defined by

$$\mathbf{N}(\xi) = \mathbf{A} + \mathbf{U}(\xi\mathbf{I} - \mathbf{V})^{-1}\mathbf{B}, \quad \xi \in \mathbb{C} - \sigma(\mathbf{V}). \tag{2.17}$$

Here, $\sigma(\mathbf{V})$ stands for the spectrum of the matrix $\mathbf{V}$. This terminology of the Nyquist stability function was suggested by Hill [18], although this function in the context of GLMs was first introduced by Butcher [4], who did not assign to it any specific name.

Denote by $\widetilde{\mathbf{w}}$ a principal left eigenvector of $\mathbf{V}$, i.e., the vector such that

$$\widetilde{\mathbf{w}}^T\mathbf{V} = \widetilde{\mathbf{w}}^T, \quad \widetilde{\mathbf{w}}^T\mathbf{q}_0 = 1, \tag{2.18}$$

where $\mathbf{q}_0$ is the preconsistency vector of GLM (2.2). Following [18] define the diagonal matrix $\widetilde{\mathbf{D}}$ by

$$\widetilde{\mathbf{D}} = \operatorname{diag}(\mathbf{B}^T\widetilde{\mathbf{w}}), \tag{2.19}$$

and following [4], define by $\operatorname{He}(\mathbf{Q})$ the Hermitian part of a complex square matrix $\mathbf{Q}$, i.e.,

$$\operatorname{He}(\mathbf{Q}) = \frac{1}{2}\Big(\mathbf{Q} + \mathbf{Q}^*\Big),$$

where $\mathbf{Q}^*$ stands for the conjugate transpose of $\mathbf{Q}$. Then it was demonstrated in [4] and [18] 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. $\widetilde{\mathbf{D}} > 0$ and $\operatorname{He}(\widetilde{\mathbf{D}}\mathbf{A}) \geq 0$.
4. $\operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi)) \geq 0$ for all ξ such that $|\xi| = 1$ and $\xi \in \mathbb{C} - \sigma(\mathbf{V})$.

The numerical search for algebraically stable TSRK methods with $\vartheta = 0$, $u = 0$ and $\vartheta \neq 0$, $u \neq 0$, which is based on the criterion consisting of the conditions 1–4 is described in the next two sections.

3. TSRK methods with $\vartheta = 0$ and $u = 0$.

In this section we consider TSRK methods with $\vartheta = 0$ and $u = 0$. Then putting

$$z^{[n]} = \begin{bmatrix} y_n \\ hf(Y^{[n]}) \end{bmatrix},$$

the TSRK method (1.2) can be represented as GLM (2.2) with coefficient matrices **A**, **U**, **B** and **V** defined by

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} A & e & B \\ \hline v^T & 1 & w^T \\ I & 0 & 0 \end{array}\right]. \tag{3.1}$$

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

$$p(\eta, z) = \eta^{s+1} - R_1(z)\eta^s + R_2(z)\eta^{s-1} + \cdots + (-1)^s R_s(z)\eta + (-1)^{s+1} R_{s+1}(z), \tag{3.2}$$

where $R_i(z)$ are rational functions

$$R_i(z) = \frac{p_i(z)}{p_0(z)}, \quad i = 1, 2, \ldots, s+1,$$

with

$$p_0(z) = 1 + p_{01}z + \cdots + p_{0s}z^s, \;\; p_1(z) = 1 + p_{11}z + \cdots + p_{1s}z^s,$$
$$p_2(z) = p_{21}z + \cdots + p_{2s}z^s, \;\; \ldots \;, \;\; p_s(z) = p_{s,s-1}z^{s-1} + p_{ss}z^s, \;\; p_{s+1}(z) = p_{s+1,s}z^s.$$

To investigate stability properties of GLMs (3.1) it is more convenient to work with the polynomial

$$\widetilde{p}(\eta, z) = p_0(z)p(\eta, z) \tag{3.3}$$

instead of the rational function $p(\eta, z)$ and we will always adopt this approach. The GLM (2.2) is A-stable if $\widetilde{p}(\eta, z)$ is a Schur polynomial, i.e., if the roots $\eta_i(z)$, $i = 1, 2, \ldots, s+1$, of $\widetilde{p}(\eta, z)$ are in the unit disk for all z such that $Re(z) < 0$. It follows from the maximum principle that this is the case if the roots of $p_0(z)$ are in the positive half plane $\mathbb{C}^+ = \{z : \operatorname{Re}(z) > 0\}$ and $\widetilde{p}(\eta, iy)$ is a Schur polynomial for $y \in \mathbb{R}$. This last condition can be investigated using the Schur criterion [23] as explained in [19].

It can be verified that for TSRK method (3.1) the preconsistency vector $\mathbf{q}_0$ takes the form

$$\mathbf{q}_0 = \left[\begin{array}{c} 1 \\ \hline \mathbf{0} \end{array}\right] \in \mathbb{R}^{s+1}$$

and the vector $\widetilde{\mathbf{w}}$ satisfying (2.18) is

$$\widetilde{\mathbf{w}} = \left[\begin{array}{c} 1 \\ \hline w \end{array}\right] \in \mathbb{R}^{s+1}.$$

Hence, the matrix $\widetilde{\mathbf{D}}$ defined by (2.19) takes the form

$$\widetilde{\mathbf{D}} = \operatorname{diag}\left(\left[\begin{array}{c|c} v & I \end{array}\right]\left[\begin{array}{c} 1 \\ \hline w \end{array}\right]\right) = \operatorname{diag}(v + w).$$

We next compute the Nyquist stability function $\mathbf{N}(\xi)$ corresponding to TSRK method (3.1) and the Hermitian part of $\widetilde{\mathbf{D}}\mathbf{N}(\xi)$. Using the formula

$$\left[\begin{array}{c|c} A & B \\ \hline 0 & D \end{array}\right]^{-1} = \left[\begin{array}{c|c} A^{-1} & -A^{-1}BD^{-1} \\ \hline 0 & D^{-1} \end{array}\right],$$

where A and D are square and nonsingular matrices, we have

$$\mathbf{N}(\xi) = A + \left[\begin{array}{c|c} e & B \end{array}\right] \left[\begin{array}{c|c} \xi - 1 & -w^T \\ \hline 0 & \xi I \end{array}\right]^{-1} \left[\begin{array}{c} v^T \\ \hline I \end{array}\right] = A + \frac{1}{1-\xi}\, e\, v^T + \frac{1}{\xi(\xi-1)}\, e\, w^T + \frac{1}{\xi} B\,,$$

and taking into account that

$$\widetilde{\mathbf{D}}e = \operatorname{diag}(v+w)e = v + w, \quad e^T\widetilde{\mathbf{D}} = e^T \operatorname{diag}(v+w) = (v+w)^T,$$

it follows that

$$\begin{aligned}\operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi)) \;\;=\;\; & \frac{1}{2}\Big(\widetilde{\mathbf{D}}\big(A + \frac{1}{\xi}B\big) + \big(A^T + \frac{1}{\overline{\xi}}B^T\big)\widetilde{\mathbf{D}} + \big(\frac{1}{\xi-1} + \frac{1}{\overline{\xi}-1}\big)vv^T + \big(\frac{1}{\overline{\xi}-1} + \frac{1}{\xi(\xi-1)}\big)vw^T \\ & + \big(\frac{1}{\xi-1} + \frac{1}{\overline{\xi}(\overline{\xi}-1)}\big)wv^T + \big(\frac{1}{\xi(\xi-1)} + \frac{1}{\overline{\xi}(\overline{\xi}-1)}\big)ww^T\Big),\end{aligned}$$

where $\overline{\xi}$ stands for conjugate of ξ. We next compute the limit

$$\lim_{t\to 0} \operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}}.$$

Since

$$\lim_{t\to 0}\big(\frac{1}{\xi-1} + \frac{1}{\overline{\xi}-1}\big)\Big|_{\xi=e^{it}} = -1, \quad \lim_{t\to 0}\big(\frac{1}{\overline{\xi}-1} + \frac{1}{\xi(\xi-1)}\big)\Big|_{\xi=e^{it}} = -2,$$

$$\lim_{t\to 0}\big(\frac{1}{\xi-1} + \frac{1}{\overline{\xi}(\overline{\xi}-1)}\big)\Big|_{\xi=e^{it}} = -2, \quad \lim_{t\to 0}\big(\frac{1}{\xi(\xi-1)} + \frac{1}{\overline{\xi}(\overline{\xi}-1)}\big)\Big|_{\xi=e^{it}} = -3,$$

it follows that

$$\lim_{t\to 0} \operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} = \frac{1}{2}\Big(\operatorname{diag}(v+w)(A+B) + (A+B)^T\operatorname{diag}(v+w) - vv^T - 2(vw^T + wv^T) - 3ww^T\Big). \tag{3.4}$$

Observe also that $\operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ does not have a limit as $\xi \to 1$. For example, as $\xi = x \to 1$ along the real axis we have

$$\lim_{x\to 1} \operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=x} = \infty.$$

4. TSRK methods with $\vartheta \neq 0$ and $u \neq 0$.

We now consider the general case where $\vartheta \neq 0$ and $u \neq 0$. Similarly as in Section 3, putting

$$z^{[n]} = \begin{bmatrix} y_n \\ y_{n-1} \\ hf(Y^{[n]}) \end{bmatrix},$$

the TSRK method (1.2) can be represented as GLM (2.2) with coefficient matrices $\mathbf{A}$, $\mathbf{U}$, $\mathbf{B}$ and $\mathbf{V}$ defined by

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|ccc} A & e-u & u & B \\ \hline v^T & 1-\vartheta & \vartheta & w^T \\ 0 & 1 & 0 & 0 \\ I & 0 & 0 & 0 \end{array}\right]. \tag{4.1}$$

Similarly as in Section 3 it can be verified that the stability function $p(\eta, z)$ of this method takes the form

$$p(\eta, z) = \eta^{s+2} - R_1(z)\eta^{s+1} + R_2(z)\eta^s + \cdots + (-1)^{s+1}R_{s+1}(z)\eta + (-1)^{s+2}R_{s+2}(z), \tag{4.2}$$

where $R_i(z)$ are rational functions

$$R_i(z) = \frac{p_i(z)}{p_0(z)}, \quad i = 1, 2, \ldots, s+2,$$

with

$$p_0(z) = 1 + p_{01}z + \cdots + p_{0s}z^s, \ \ p_1(z) = 1 - \vartheta + p_{11}z + \cdots + p_{1s}z^s,$$
$$p_2(z) = -\vartheta + p_{21}z + \cdots + p_{2s}z^s, \ \ \ldots\ , \ \ p_{s+1}(z) = p_{s+1,s-1}z^{s-1} + p_{s+1,s}z^s, \ \ p_{s+2}(z) = p_{s+2,s}z^s.$$

As before, to investigate stability properties of GLMs (4.1) it is more convenient to work with the polynomial $\widetilde{p}(\eta, z) = p_0(z)p(\eta, z)$ instead of the rational function $p(\eta, z)$ and we will again always adopt this approach.

Similarly as in Section 3 it can be verified that for TSRK method (4.1) the preconsistency vector $\mathbf{q}_0$ takes the form

$$\mathbf{q}_0 = \begin{bmatrix} 1 \\ 1 \\ \mathbf{0} \end{bmatrix} \in \mathbb{R}^{s+2},$$

the vector $\widetilde{\mathbf{w}}$ satisfying (2.18) is

$$\widetilde{\mathbf{w}} = \frac{1}{1+\vartheta}\begin{bmatrix} 1 \\ \vartheta \\ w \end{bmatrix} \in \mathbb{R}^{s+2},$$

and the matrix $\widetilde{\mathbf{D}}$ defined by (2.19) is

$$\widetilde{\mathbf{D}} = \frac{1}{1+\vartheta}\operatorname{diag}(v+w).$$

The following result holds and its proof is reported in [10],

$$\begin{aligned}\lim_{t\to 0}\operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} = \frac{1}{2(1+\vartheta)}\Big(&\operatorname{diag}(v+w)\big(A+B\big) + (A+B)^T\operatorname{diag}(v+w) - \frac{1-\vartheta}{(1+\vartheta)^2}vv^T - \frac{3+\vartheta}{(1+\vartheta)^2}ww^T \\ &- \frac{2}{(1+\vartheta)^2}(vw^T + wv^T) - \frac{1}{1+\vartheta}\Big(((v+w)\cdot u)(v+w)^T + (v+w)((v+w)\cdot u)^T\Big)\Big).\end{aligned}$$

Observe that for $\vartheta = 0$ and $u = 0$ this formula for $\lim_{t\to 0}\operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ reduces to the formula obtained in Section 3.

5. Examples of TSRK methods with $\vartheta = 0$ and $u = 0$.

We have implemented an algorithm for numerical search for algebraically stable TSRK methods written as GLMs (3.1). This algorithm is based on minimizing the objective function which computes the negative value of the minimum of the eigenvalues of the matrix $\operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ for ξ such that $|\xi| = 1$ and $\xi \in \mathbb{C} - \sigma(\mathbf{V})$. This objective function is a numerical realization of the necessary condition 4 for algebraic stability, which is listed at the end of Section 2. Once the methods for which $\operatorname{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi)) \geq 0$ for ξ such that $|\xi| = 1$ and $\xi \in \mathbb{C} - \sigma(\mathbf{V})$ are found, the remaining necessary conditions 1-3 for algebraic stability are verified on the case by case basis.

In what follows we will present the results of our search for A-stable and algebraically stable methods (3.1) with the number of stages $s = 1$, $s = 2$, and $s = 3$.

1. Methods with $s = 1$, $p = 2$, and $q = 2$. Solving stage order and order conditions

$$C_k = 0, \quad \widetilde{C}_k = 0, \quad k = 1, 2,$$

we obtain a one-parameter family of methods of order $p = 2$ and stage order $q = 2$ with coeffcients given by

$$\begin{array}{c|c|c} u & A & B \\ \hline \vartheta & v & w \end{array} = \begin{array}{c|c|c} 0 & \frac{c(2-c)}{2} & \frac{c^2}{2} \\ \hline 0 & \frac{3-2c}{2} & \frac{2c-1}{2} \end{array},$$

where c is the abscissa. These methods are not algebraically stable for any c and are A-stable only if $c = 1$, for which the resulting method is equivalent to the trapezoidal rule

$$y_n = y_{n-1} + \frac{h}{2}\Big(f(y_{n-1}) + f(y_n)\Big).$$

2. Methods with $s = 1$, $p = 2$, and $q = 1$. Solving stage order and order conditions

$$C_1 = 0, \quad \widetilde{C}_1 = 0, \quad \widetilde{C}_2 = 0,$$

we obtain a two-parameter family of methods of order $p = 2$ and stage order $q = 1$ depending on a and c. The coeffcients of these methods are given by

$$\begin{array}{c|c|c} u & A & B \\ \hline \vartheta & v & w \end{array} = \begin{array}{c|c|c} 0 & a & c-a \\ \hline 0 & \frac{3-2c}{2} & \frac{2c-1}{2} \end{array}.$$

It can be verified using the Schur criterion discussed in Section 3 that these methods are A-stable if $a \geq 1/2$. It can be also verified using the approach based on Albert theorem described in Section 2 that the conditions (2.13), (2.14) and (2.16) are satisfied if

$$g_{22} > 0 \quad \text{and} \quad 0 < \frac{g_{11}}{g_{22}} < \frac{4}{1 - 4c + 4c^2} \quad \text{and} \quad a = \frac{1 + 4c - 4c^2}{4} + \frac{g_{22}}{g_{11}}.$$

This implies that these methods are algebraically stable if $a > 1/2$. Puttting, for example, $c = 3/4$ and $a = 1$ we obtain the method

$$\begin{array}{c|c|c} u & A & B \\ \hline \vartheta & v & w \end{array} = \begin{array}{c|c|c} 0 & 1 & -\frac{1}{4} \\ \hline 0 & \frac{3}{4} & \frac{1}{4} \end{array}$$

for which the matrix $\mathbf{M}$ defined in Section 2 is nonnegative definite if we choose

$$\mathbf{G} = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} = \begin{bmatrix} 1 & \frac{1}{4} \\ \frac{1}{4} & \frac{9}{16} \end{bmatrix}, \quad \mathbf{D} = 1.$$

This confirm again that this particular TSRK method is algebraically stable.

3. Methods with $s = 2$, $p = 4$, and $q = 4$. Solving stage order and order conditions

$$C_k = 0, \quad \widetilde{C}_k = 0, \quad k = 1, 2, 3, 4,$$

we obtain a two-parameter family of methods of order $p = 4$ and stage order $q = 4$ depending on the components of the abscissa vector c_1 and c_2. The coefficients of these methods are not listed here. However, we were not able to find the methods which are algebraically stable or A-stable and we suspect that such methods do not exist in this class.

4. Methods with $s = 2$, $p = 4$, and $q = 3$. Solving stage order and order conditions

$$C_k = 0, \quad k = 1, 2, 3, \quad \widetilde{C}_k = 0, \quad k = 1, 2, 3, 4,$$

we obtain a four-parameter family of methods of order $p = 4$ and stage order $q = 3$ depending on c_1, c_2, a_{12} and a_{22}. The stability polynomial $\widetilde{p}(\eta, z)$ defined by (3.3) takes the form

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

where

$$p_0(z) = 1 + p_{01}z + p_{02}z^2, \quad p_1(z) = 1 + p_{11}z + p_{12}z^2, \quad p_2(z) = p_{21}z + p_{22}z^2, \quad p_3(z) = p_{31}z^2.$$

In our search for A-stable methods we compute first the parameter a_{22} from the algebraic equation

$$p_{31} = 0$$

and then apply the Schur criterion discussed in Section 3 to the quadratic polynomial

$$p_0(z)\eta^2 - p_1(z)\eta + p_2(z).$$

The results of this search are presented in Fig. 1 in the parameter space (c_1, c_2) for selected values of the parameter a_{12}, and in Fig. 2 in the parameter space (c_1, a_{12}) for $c_2 = 1$.

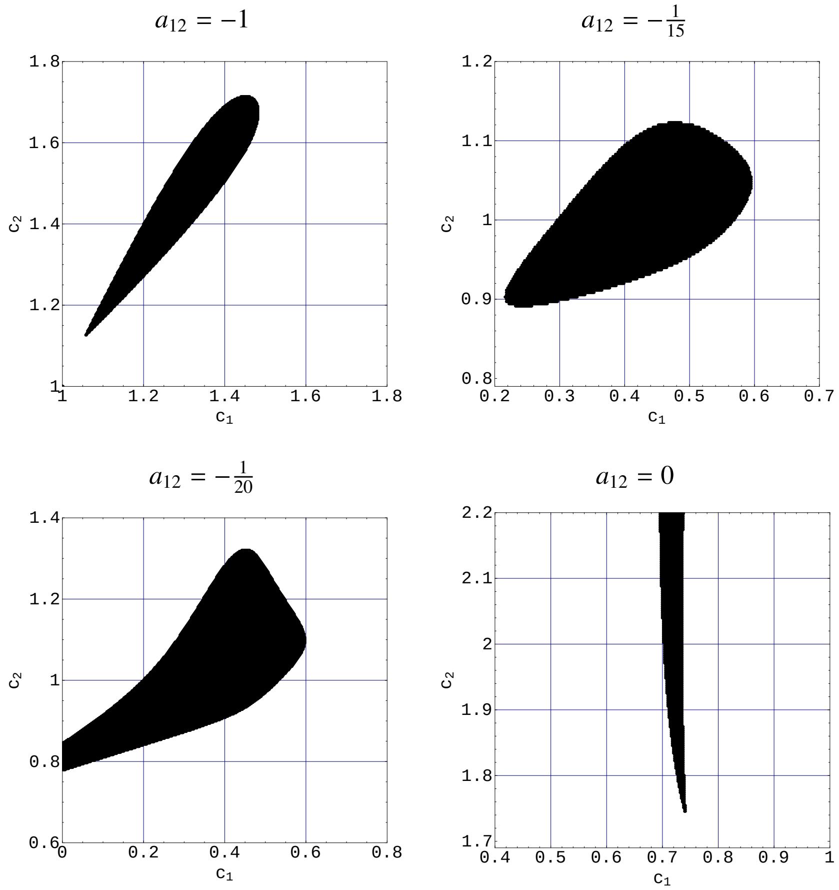

Figure 1: Regions of A-stability in the parameter space (c_1, c_2) for TSRK methods with $p = 4$ and $q = 3$, for specific values of a_{12}.

We will next search for algebraically stable methods using the conditions 1–4 listed at the end of Section 2. This search is based on minimizing the negative value of the objective function which computes the minimum of the eigenvalues of the matrix $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))|_{\xi=e^{it}}$ for $t \in [0, 2\pi]$. It can be verified using formula (3.4) that

$$\lim_{t\to 0} \det\left(\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}}\right) = -\frac{F(c_1, c_2, a_{12}, a_{22})^2}{(c_1 - c_2)^2(c_1 - c_2 - 1)^4(c_1 - c_2 + 1)^4},$$

where $F(c_1, c_2, a_{12}, a_{22})$ is a polynomial with respect to c_1, c_2, a_{12}, a_{22}. To satisfy the condition 4 at the end of Section 2, i.e.,

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi)) \geq 0, \quad |\xi| = 1, \quad \xi \in \mathbb{C} - \sigma(\mathbf{V}),$$

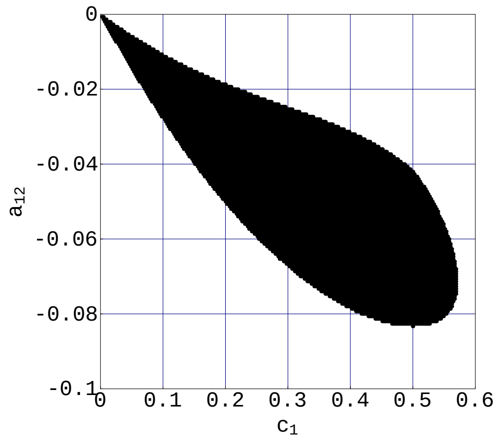

Figure 2: Region of A-stability in the parameter space (c_1, a_{12}) for TSRK methods methods with $p = 4$ and $q = 3$ for $c_2 = 1$.

for $\xi = 1$ or $t = 0$, $t = 2\pi$, we compute the parameter a_{12} from the equation

$$F(c_1, c_2, a_{12}, a_{22}) = 0. \tag{5.1}$$

The search in the parameter space (c_1, c_2, a_{22}) did not lead to any methods which are algebraically stable. We were only able to find methods for which

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq -2.68 \cdot 10^{-3}, \tag{5.2}$$

$t \in [0, 2\pi]$. Not imposing the condition (5.1) and searching in the parameter space $(c_1, c_2, a_{12}, a_{22})$ we were able to find some algebraically stable methods but, unfortunately, with unrealistically large values of some parameters c_1, c_2, a_{12}, or a_{22}. Restricting this search to $0 \leq c_1, c_2 \leq 1$, $-1 \leq a_{12}, a_{22} \leq 1$ we found methods for which

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq -5.28 \cdot 10^{-4}, \tag{5.3}$$

$t \in [0, 2\pi]$.

5. Methods with $s = 3$, $p = 4$, and $q = 4$. Solving stage order and order conditions

$$C_k = 0, \quad \widetilde{C}_k = 0, \quad k = 1, 2, 3, 4,$$

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 (3.3) for this family of methods takes the form

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

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. 3 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

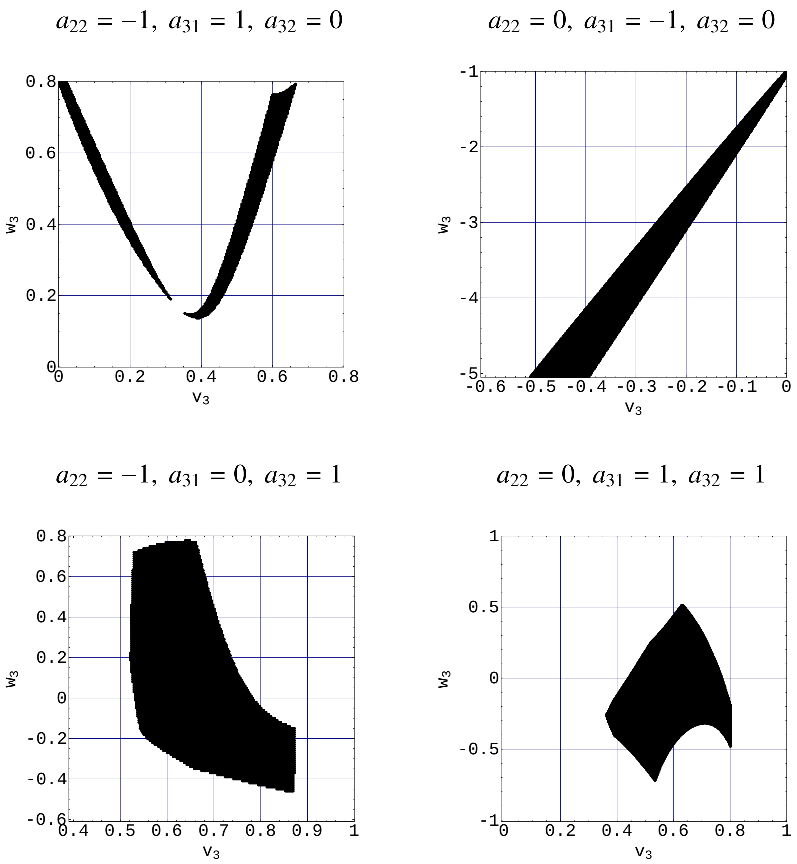

Figure 3: Regions of A-stability in the (v_3, w_3)-plane, for TSRK methods with $s = 3$ and $p = q = 4$, for specific values of the parameters a_{22}, a_{31}, a_{32}.

general abscissa vector c. Although we did not find such methods, we found formulas for which

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq -3.50 \cdot 10^{-11}, \tag{5.4}$$

$t \in [0, 2\pi]$. 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 coeffcients of a method satisfying (5.4) are

$$c = \begin{bmatrix} 0.748023646320140 & -0.088623514454709 & 1.356515696201252 \end{bmatrix}^T,$$

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

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

$$v = \begin{bmatrix} 0.622394316996030 & 0.313242750536090 & -0.011784503142076 \end{bmatrix}^T,$$

$$w = \begin{bmatrix} -0.062831671181596 & -0.008857653267082 & 0.147836760058631 \end{bmatrix}^T.$$

6. Methods with $s = 3$, $p = 4$, and $q = 3$. Solving stage order and order conditions

$$C_k = 0, \quad k = 1, 2, 3, \quad \widetilde{C}_k = 0, \quad k = 1, 2, 3, 4,$$

we obtain an eleven-parameter family of methods of order $p = 4$ and stage order $q = 3$ depending on a_{ij}, $i, j = 1, 2, 3$, v_3, and w_3. In our search for A-stable methods we assume again that $c = [0, 1/2, 1]^T$. We compute the parameters a_{11}, a_{12}, and a_{13} to reduce the degree of stability polynomal to 3. As a result we obtain an eight-parameter family of methods depending on a_{21}, a_{22}, a_{23}, a_{31}, a_{32}, a_{33}, v_3, and w_3. The result of this search are produced on Fig. 4. The

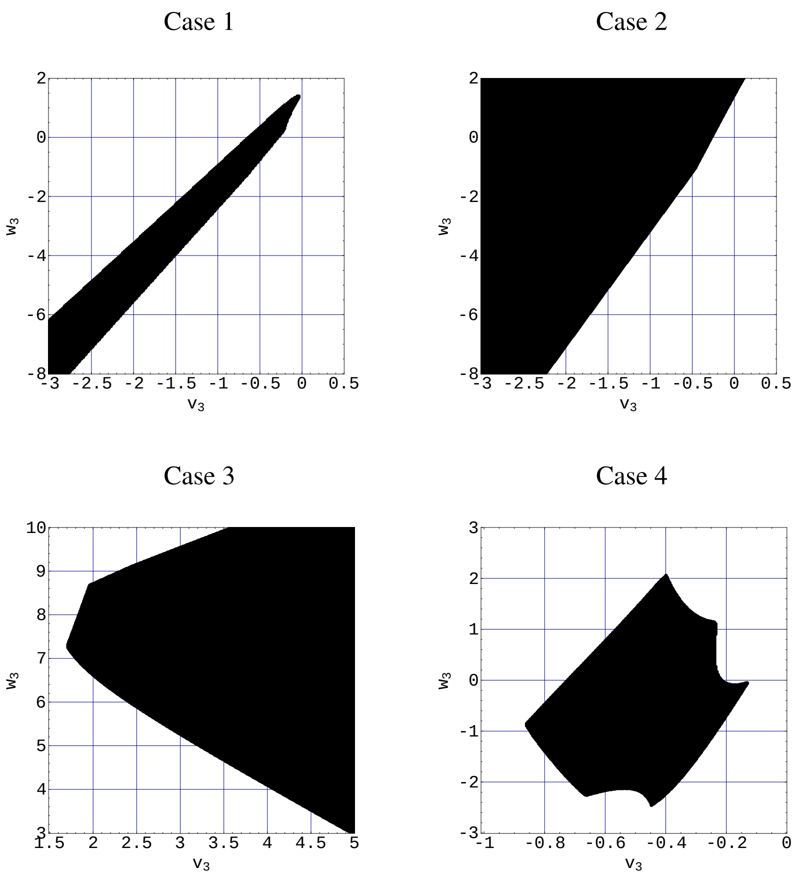

Figure 4: Regions of A-stability in the (v_3, w_3)-plane, for TSRK methods with $s = 3$ and $p = q = 4$ for specific values of the parameters

four cases in Fig. 4 correspond to:

- Case 1: $a_{21} = 2/3, a_{22} = 1, a_{23} = 1, a_{31} = -1/3, a_{32} = -1, a_{33} = 1/2$.
- Case 2: $a_{21} = 2, a_{22} = 1/2, a_{23} = 1, a_{31} = 1, a_{32} = -1, a_{33} = 1$.
- Case 3: $a_{21} = 2, a_{22} = 1, a_{23} = 1, a_{31} = 0, a_{32} = 1, a_{33} = 1$.
- Case 4: $a_{21} = 2, a_{22} = 1/2, a_{23} = 1/2, a_{31} = 1, a_{32} = 1/4, a_{33} = 1$.

In our search for algebraically stable methods, we found formulas for which

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq -3.77 \cdot 10^{-11}, \tag{5.5}$$

$t \in [0, 2\pi]$. As before, 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 coeffcients of a method satisfying (5.5) are

$$c = \begin{bmatrix} 0 & \frac{9}{10} & \frac{1}{5} \end{bmatrix}^T,$$

$$A = \begin{bmatrix} 1.923612711387117 & 0.332510317035363 & -2.361485324294705 \\ -0.042296580010526 & 0.264934173014572 & 0.753491461692750 \\ -0.754264567991751 & -0.285410192009791 & 1.590352848308200 \end{bmatrix},$$

$$B = \begin{bmatrix} -0.059505325459301 & 0.350609358761479 & -0.185741737429953 \\ 0.035823298712475 & -0.054110902952294 & -0.057841450456976 \\ 0.583885022389948 & -0.292809804314522 & -0.641753306382084 \end{bmatrix},$$

$$v = \begin{bmatrix} 0.085993246200685 & 0.374327773490317 & 0.659375459065431 \end{bmatrix}^T,$$

$$w = \begin{bmatrix} 0.123800116578393 & -0.056810353776912 & -0.186686241557912 \end{bmatrix}^T.$$

6. Examples of TSRK methods with $\vartheta \neq 0$ and $u \neq 0$.

As in Section 5, we will use Schur criterion to search for A-stable TSRK methods, and the criterion based on conditions 1-4 listed at the end of Section 2 to search for TSRK methods which are algebraically stable. In the remainder of this section we will present the results of our search for such methods (4.1) with the number of stages $s = 1$, $s = 2$, and $s = 3$.

1. Methods with $s = 1$, $p = 2$, and $q = 2$. Assuming that $\mathbf{c} = c_1 = 1$ and solving stage order and order conditions

$$C_k = 0, \quad \widetilde{C}_k = 0, \quad k = 1, 2,$$

we obtain a two-parameter family of methods of order $p = 2$ and stage order $q = 2$ with coeffcients given by

$$\begin{array}{c|c|c} u & A & B \\ \hline \vartheta & v & w \end{array} = \begin{array}{c|c|c} u & \frac{1-u}{2} & \frac{1+3u}{2} \\ \hline \vartheta & \frac{1-\vartheta}{2} & \frac{1+3\vartheta}{2} \end{array}.$$

It can be verified using Schur criterion that these methods are A-stable if and only if

$$-1 < \vartheta < 0 \quad \text{and} \quad \frac{\vartheta(\vartheta+3)}{2(\vartheta+1)} \leq u \leq \frac{\vartheta}{2}$$

or $u = \vartheta = 0$. The last case corresponds again to the trapezoidal rule obtained in Section 5.

To search for methods which are algebraically stable we use the criteria (2.15) or (2.16) based on Albert's theorem discussed in Section 2. The example of such a method is given by

$$\begin{array}{c|c|c} u & A & B \\ \hline \vartheta & v & w \end{array} = \begin{array}{c|c|c} -\frac{3}{4} & \frac{7}{8} & -\frac{5}{8} \\ \hline -\frac{1}{2} & \frac{3}{4} & -\frac{1}{4} \end{array}.$$

We can verify that choosing positive definite matrices $\mathbf{G}$ and $\mathbf{D}$,

$$\mathbf{G} = \begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix} = \begin{bmatrix} \frac{14}{13} & -\frac{9}{13} & -\frac{21}{52} \\ -\frac{9}{13} & \frac{1}{2} & \frac{4}{13} \\ -\frac{21}{52} & \frac{4}{13} & \frac{27}{104} \end{bmatrix}, \quad \mathbf{D} = \begin{bmatrix} \frac{5}{26} \end{bmatrix},$$

the matrix $\mathbf{M}$ defined in Section 2 is nonnegative definite.

2. Methods with $s = 2$, $p = 4$, and $q = 4$. Solving stage order and order conditions

$$C_k = 0, \quad \widetilde{C}_k = 0, \quad k = 1,2,3,4,$$

we obtain a five-parameter family of methods of order $p = 4$ and stage order $q = 4$ depending on c_1, c_2, u_1, u_2, and ϑ. In our search for A-stable methods we computed first ϑ, u_1, and u_2 to reduce the degree of stability polynomial from 4 to 2. As a consequence we obtain a two-parameter family of methods depending on c_1 and c_2. The results of computer search are presented on Fig. 5.

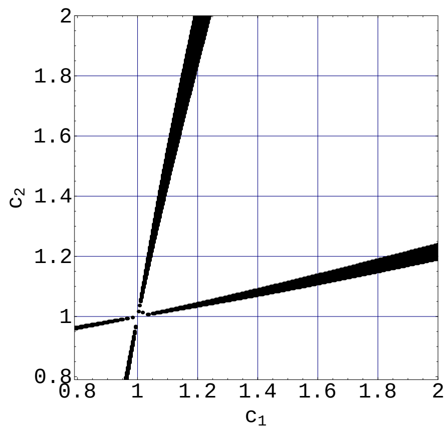

Figure 5: Regions of A-stability and in the (c_1, c_2)-plane, for TSRK methods with $s = 2$ and $p = q = 4$

We were not able to find algebraically stable methods in this class, and the best bound we were able to satisfy is

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq -2.89 \cdot 10^{-3},$$

$t \in [0, 2\pi]$.

3. Methods with $s = 2$, $p = 4$, and $q = 3$. Solving stage order and order conditions

$$C_k = 0, \quad k = 1,2,3, \quad \widetilde{C}_k = 0, \quad k = 1,2,3,4,$$

we obtain a seven-parameter family of methods of order $p = 4$ and stage order $q = 3$ depending on c_1, c_2, a_{12}, a_{22}, u_1, u_2, and ϑ. To search for A-stable methods we assume that $c = [1/2, 1]^T$. We next determine ϑ to reduce the degree of $\widetilde{p}(\eta, z)$ from 4 to 3. This leads to a four-parameter family of methods depending on a_{12}, a_{22}, u_1, and u_2. The results of the search are presented in Fig 6 for selected values of the parameters u_1 and u_2.

As in the previous case, we were not able to find algebraically stable methods in this class, and the best bound we were able to satisfy is

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq -7.70 \cdot 10^{-8},$$

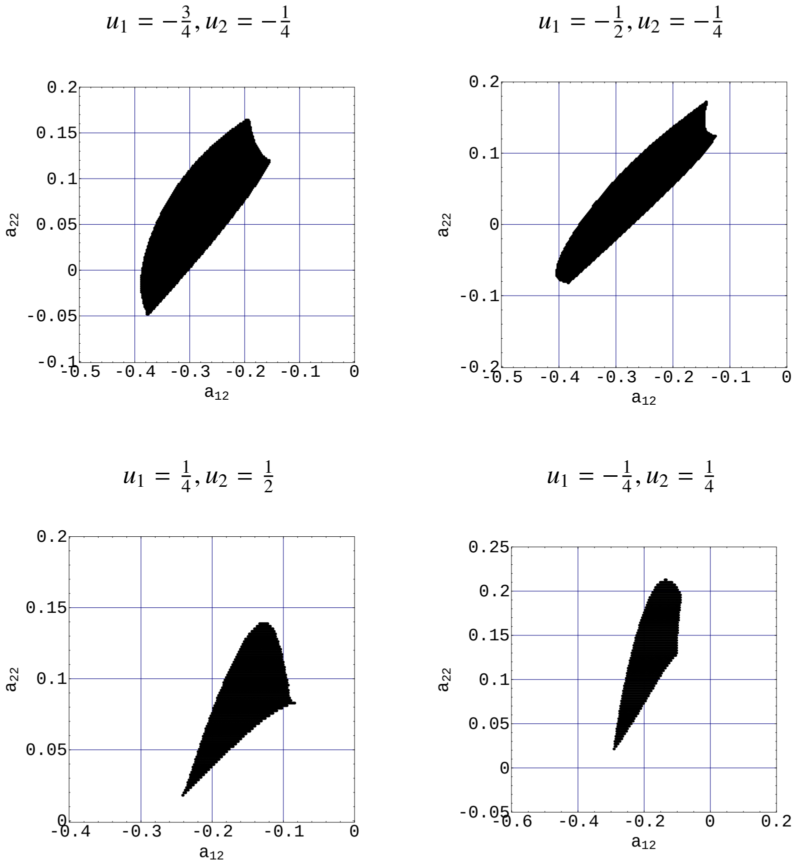

Figure 6: Regions of A-stability in the (a_{12}, a_{22})-plane, for TSRK methods with $s = 2$, $p = 4$, and $q = 3$, for specific values of the parameters u_1 and u_2.

$t \in [0, 2\pi]$. The coeffcients of a method corresponding to this bound are $\vartheta = 0.045477710128446$,

$$c = \begin{bmatrix} 2.336580469857886 & 1.243897612851233 \end{bmatrix}^T,$$

$$u = \begin{bmatrix} -0.009140162241697 & -0.004971562691777 \end{bmatrix}^T,$$

$$A = \begin{bmatrix} 0.382519266813101 & 1.231791538880037 \\ -0.067916000101827 & 0.439694807309414 \end{bmatrix},$$

$$B = \begin{bmatrix} 0.123031161533802 & 0.590098340389249 \\ 0.161425752706173 & 0.705721490245697 \end{bmatrix},$$

$$v = \begin{bmatrix} -0.033116900308262 & -0.046491551194616 \end{bmatrix}^T,$$

$$w = \begin{bmatrix} 0.309391097083087 & 0.815695064548217 \end{bmatrix}^T.$$

We have also tried to find methods with c_1 and c_2 in the interval $[0, 1]$. We found methods for which

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq -4.42 \cdot 10^{-5},$$

$t \in [0, 2\pi]$. The coeffcients of a method corresponding to this bound are $\vartheta = 0.334852100666355$,

$$c = \begin{bmatrix} 0.817535264370424 & 0.111499700613041 \end{bmatrix}^T,$$

$$u = \begin{bmatrix} 0.381412710198958 & 0.549351922349542 \end{bmatrix}^T,$$

$$A = \begin{bmatrix} 0.261809682531266 & 0.716578941913569 \\ -0.055221137652820 & 0.331382626202203 \end{bmatrix},$$

$$B = \begin{bmatrix} 0.064452365556917 & 0.156106984567630 \\ 0.115480859585862 & 0.269209274827339 \end{bmatrix},$$

$$v = \begin{bmatrix} 0.484238639043203 & 0.651111475466369 \end{bmatrix}^T,$$

$$w = \begin{bmatrix} 0.058567341150044 & 0.140934645006739 \end{bmatrix}^T.$$

4. Methods with $s = 3$, $p = 4$, and $q = 4$. Solving stage order and order conditions

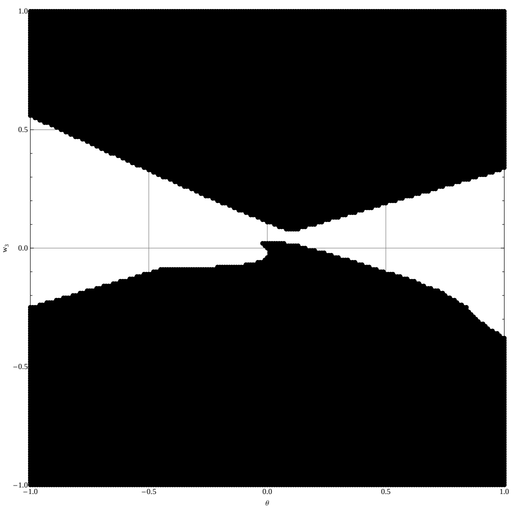

Figure 7: Regions of A- and L-stability in the (ϑ, w_3)-plane, for TSRK methods with $s = 3$, $p = 4$, and $q = 4$

$$C_k = 0, \quad \widetilde{C}_k = 0, \quad k = 1, 2, 3, 4,$$

we obtain a fifteen-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, w_3, u_1, u_2, u_3, and ϑ. We used most of these parameters to reduce the degree of stability polynomial from 5 to 3 and to acheve L-stability. In Fig. 7 we present the A- and L-stable methods in the parameter space (ϑ, w_3).

We next investigate algebraic stability. In this family we have found methods for which

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi = e^{it}} \geq 0,$$

$t \in [0, 2\pi]$, with small negative c_1 and with c_2 and c_3 in the interval $[0, 1]$. The coefficients of such a method are $\vartheta = -0.848157324846955$,

$$c = \begin{bmatrix} -0.001034365439338 & 0.460202200222726 & 0.904412078001496 \end{bmatrix}^T,$$

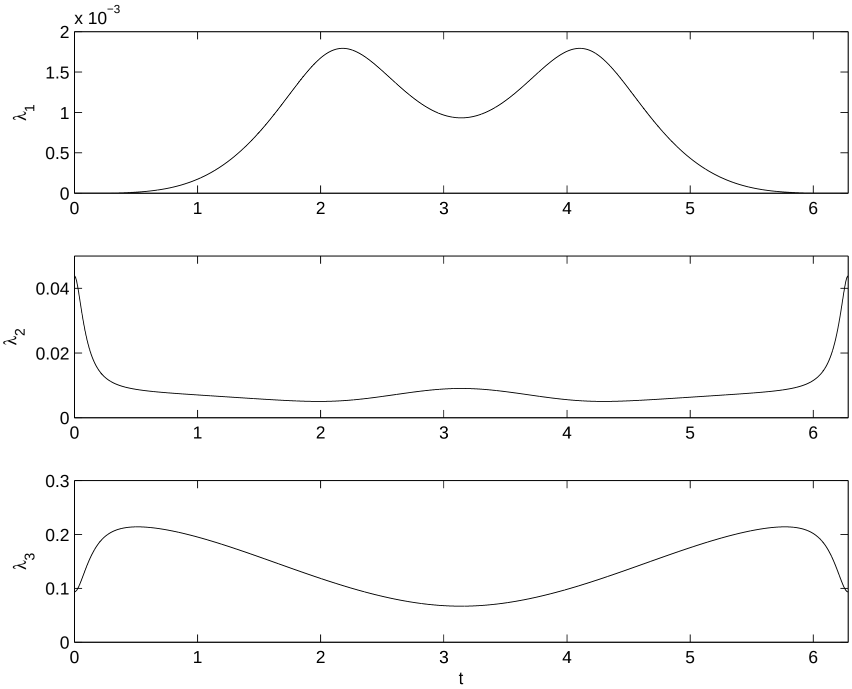

Figure 8: Eigenvalues $\lambda_1(t)$, $\lambda_2(t)$, and $\lambda_3(t)$ of the matrix $\mathrm{He}(\widetilde{\mathbf{DN}}(\xi))$ for $\xi = e^{it}$, $t \in [0, 2\pi]$

$$u = \begin{bmatrix} -4.095771377315513 & -8.224398492425298 & -1.491121282659948 \end{bmatrix}^T,$$

$$A = \begin{bmatrix} 0.313393425882524 & -0.230606333014524 & 0.057318614979789 \\ 0.145030029219694 & 0.433646707347174 & -0.082047057840003 \\ 0.298592649650861 & 0.485659580434091 & 0.175944782009046 \end{bmatrix},$$

$$B = \begin{bmatrix} -0.589101054212143 & -2.620606437887970 & -1.027203958502527 \\ -1.339460229044111 & -4.705966457621601 & -2.215399284263721 \\ -0.206836462942642 & -0.983942583478110 & -0.356127170331698 \end{bmatrix},$$

$$v = \begin{bmatrix} 0.174157205530582 & 0.575265278532646 & 0.258760729183023 \end{bmatrix}^T,$$

$$w = \begin{bmatrix} -0.135787037506238 & -0.496815665848241 & -0.223737834738728 \end{bmatrix}^T.$$

The eigenvalues $\lambda_1(t)$, $\lambda_2(t)$, and $\lambda_3(t)$ of the matrix $\mathrm{He}(\widetilde{\mathbf{DN}}(\xi))$ for $\xi = e^{it}$, $t \in [0, 2\pi]$, are plotted in Fig. 8.

5. Methods with $s = 3$, $p = 4$, and $q = 3$. Solving stage order and order conditions

$$C_k = 0, \quad k = 1, 2, 3, \quad \widetilde{C}_k = 0, \quad k = 1, 2, 3, 4,$$

we obtain an eighteen-parameter family of methods of order $p = 4$ and stage order $q = 4$ depending on c_1, c_2, c_3, a_{ij}, $i, j = 1, 2, 3$, v_3, w_3, u_1, u_2, u_3, and ϑ. Similarly as before we use most of these parameters to reduce the degree of stability polynomial from 5 to 3 and to obtain L-stability. The results of this search are presented on Fig 9 in the parameter space (ϑ, w_3) for selected values of the parameter v_3.

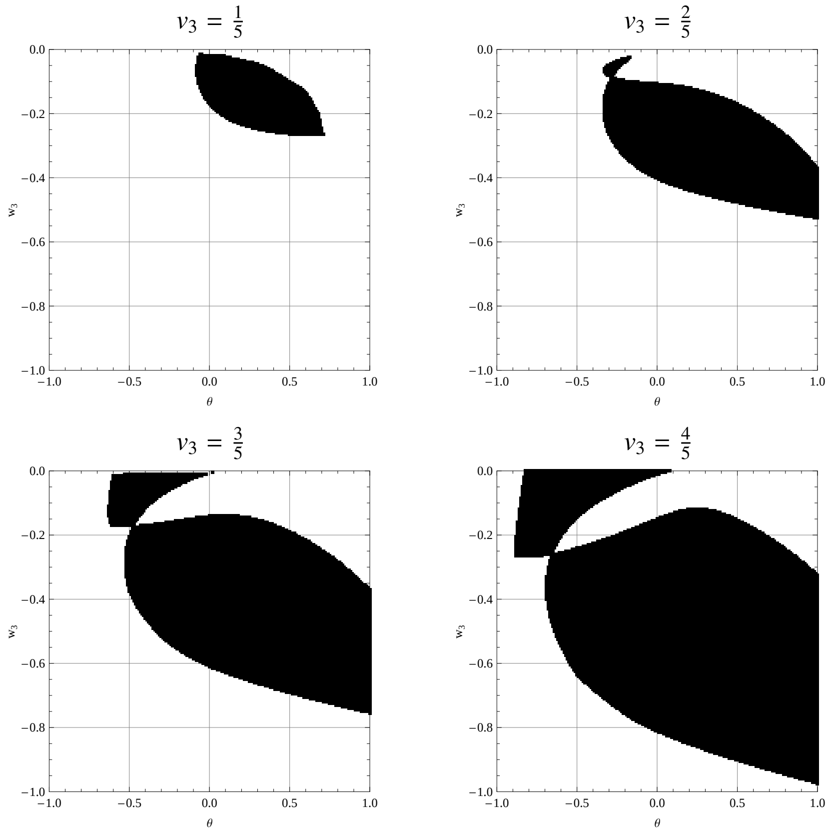

Figure 9: Regions of L-stability in the (ϑ, w_3)-plane, for TSRK methods with $s = 3$, $p = 4$, and $q = 3$, for selected values of v_3

Concerning algebraic stability, we were looking for methods with the abscissas c_1, c_2, and c_3 in the interval $[0, 1]$. We have found such methods for which

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq 0,$$

$t \in [0, 2\pi]$. The coefficients of such a method are $\vartheta = -0.564128015497646$,

$$c = \begin{bmatrix} 0.070458343197336 & 0.681445056919784 & 0.952288029979521 \end{bmatrix}^T,$$

$$u = \begin{bmatrix} -1.270302241246827 & -1.227105131502048 & -1.431550985893559 \end{bmatrix}^T,$$

$$A = \begin{bmatrix} 0.421381377377544 & -0.267169299260385 & 0.109795290241695 \\ 0.043388505707860 & 1.529849094557059 & -0.802719654220106 \\ 1.009683545410309 & -0.770029595044248 & 0.856095443003834 \end{bmatrix},$$

$$B = \begin{bmatrix} -0.319430622728631 & -1.232896302162007 & 0.088475658482292 \\ -0.184576227521167 & -1.251755340576103 & 0.120153547470190 \\ -0.633408516424409 & -0.641844792716881 & -0.299759040142642 \end{bmatrix},$$

$$v = \begin{bmatrix} 0.400771327681170 & 0.573865935770521 & 0.071538532173898 \end{bmatrix}^T,$$

$$w = \begin{bmatrix} -0.165958972572252 & -0.440020959651672 & -0.004323878899313 \end{bmatrix}^T.$$

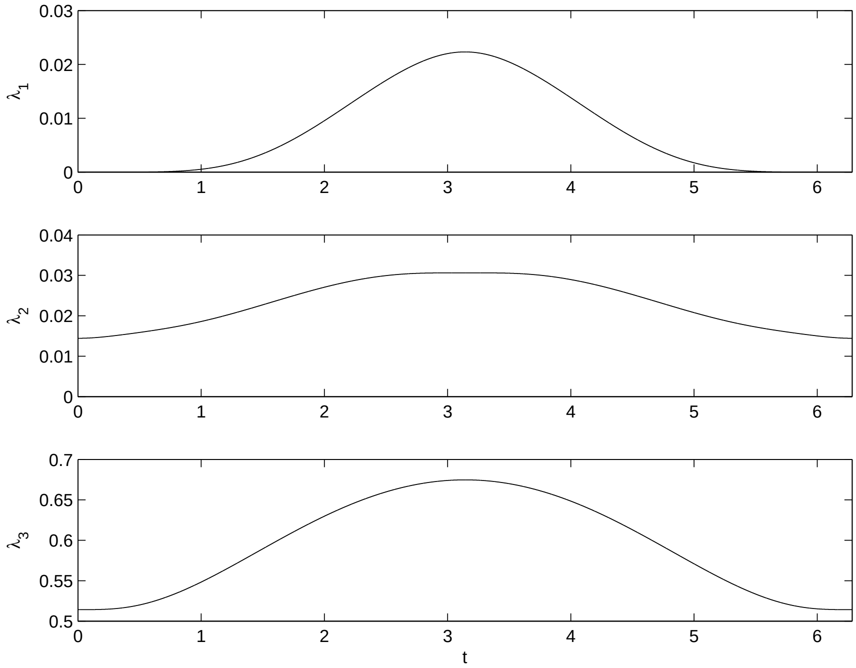

Figure 10: Eigenvalues $\lambda_1(t)$, $\lambda_2(t)$, and $\lambda_3(t)$ of the matrix $\mathrm{He}(\widetilde{\mathbf{DN}}(\xi))$ for $\xi = e^{it}$, $t \in [0, 2\pi]$

The eigenvalues $\lambda_1(t)$, $\lambda_2(t)$, and $\lambda_3(t)$ of the matrix $\mathrm{He}(\widetilde{\mathbf{DN}}(\xi))$ for $\xi = e^{it}$, $t \in [0, 2\pi]$, are plotted in Fig. 10.

7. Example of algebraically stable method of Hewitt and Hill

To put things in some perspective we analyze also the example of algebraically stable GLM of with $s = 2$, $p = 4$, and $q = 3$ constructed by Hewitt and Hill [16]. For this method the abscissa vector $\mathbf{c}$ and the coefficient matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{U}$, and $\mathbf{V}$ are given by

$$\mathbf{c} = \begin{bmatrix} 0 & \frac{193y^2-129y^4-297y^6-243y^8}{8} - \frac{1}{6} \end{bmatrix}^T,$$

$$\mathbf{A} = \begin{bmatrix} \frac{265}{864} + \frac{793y^2}{576} - \frac{5y^4}{6} - \frac{123y^6}{64} - \frac{27y^8}{16} & \frac{215}{864} - \frac{5299y^2}{576} + \frac{623y^4}{96} + \frac{915y^6}{64} + \frac{189y^8}{16} \\ \frac{101}{432} + \frac{3821y^2}{288} - \frac{463y^4}{48} - \frac{669y^6}{32} - \frac{135y^8}{8} & \frac{67}{432} + \frac{793y^2}{288} - \frac{5y^4}{3} - \frac{123y^6}{32} - \frac{27y^8}{8} \end{bmatrix},$$

$$\mathbf{B} = \begin{bmatrix} \frac{2}{3} & \frac{1}{3} \\ \frac{17y-1125y^3+828y^5+1783y^7+1458y^9}{24} & \frac{-11y+1125y^3-828y^5-1782y^7-1458y^9}{24} \end{bmatrix},$$

$$\mathbf{U} = \begin{bmatrix} 1 & -\frac{7y+9y^3}{16} \\ 0 & \frac{y+9y^3}{8} \end{bmatrix}, \quad \mathbf{V} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{bmatrix}.$$

Here $y = \pm\sqrt{z/3}$ and z is one of the two positive roots of the equation

$$9z^5 + 33z^4 + 46z^3 - 186z^2 + 9z + 1 = 0.$$

Choosing the root $z = 0.1032814360$ and $y = \sqrt{z/3}$, the decimal representation of the resulting method is

$$\mathbf{c} = [0, 0.6432188884]^T,$$

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{cc|cc} 0.3530415762 & -0.0595835887 & 1 & -0.08476931053 \\ 0.6782443859 & 0.2477498188 & 1 & 0.03037947026 \\ \hline 0.6666666667 & 0.3333333333 & 1 & 0 \\ -0.1598351741 & 0.2062215576 & 0 & 0.5 \end{array}\right].$$

It can be verified that for this method

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq -5.21 \cdot 10^{-11},$$

$t \in [0, 2\pi]$. 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, the bounds are $-1.84 \cdot 10^{-13}$ and $-1.32 \cdot 10^{-15}$, respectively.

8. Concluding remarks

We investigated A-stable and algebraically stable TSRK methods of order p and stage order $q = p$ or $q = p - 1$. These methods are first reformulated as GLMs with abscissa vector $\mathbf{c}$ and coefficient matrices $\mathbf{A}$, $\mathbf{U}$, $\mathbf{B}$ and $\mathbf{V}$. We use Schur criterion applied to the stability function $p(\eta, z) = \det(\eta\mathbf{I} - \mathbf{S}(z))$, where $\mathbf{S}(z) = \mathbf{V} + z\mathbf{B}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{U}$, is the stability matrix of the method, to search for methods which are A-stable. We use the criteria proposed recently by Hill [18] and Hewitt and Hill [16], [17] to search for algebraically stable methods. Examples of highly stable methods with $s = p$ and $q = p$ and $q = p - 1$ are given for $s = 1$, 2, and 3.

Future work will address the construction of TSRK methods of order $p = s$ and stage order $q = p$ up to order 8.

Acknowledgements. The results reported in this paper were obtained during the visits of the first two authors (RDA and GI) to the Arizona State University in 2009. These authors wish to express their gratitude to the Department of Mathematics for hospitality during these visits. We would also like to thank the referee for his useful comments.

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