Numerical search for algebraically stable two-step almost collocation methods

Dajana Conte[a], Raffaele D'Ambrosio[a], Zdzislaw Jackiewicz[b,c], Beatrice Paternoster[a]

[a]*Department of Mathematics, University of Salerno - Fisciano (Italy)*
[b]*Arizona State University - Tempe, USA*
[c]*AGH University of Science and Technology - Kraków, Poland*

Abstract

We investigate algebraic stability of the new class of two-step almost collocation methods for ordinary differential equations. These continuous methods are obtained by relaxing some of the interpolation and collocation conditions to achieve strong stability properties together with uniform order of convergence on the whole interval of integration. We describe the search for algebraically stable methods using the criterion based on the Nyquist stability function proposed recently by Hill. This criterion leads to a minimization problem in one variable which is solved using the subroutine `fminsearch` from MATLAB. Examples of algebraically stable methods in this class are also presented.

Key words: two-step Runge-Kutta methods, collocation, A-, L-, and G-stability, algebraic stability

1. Introduction

Consider the initial value problem for systems of ordinary differential equations (ODEs)

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

where the function $f : \mathbb{R}^d \to \mathbb{R}^d$ is sufficiently smooth. Concerning the numerical solution of the problem (1.1), some recent work in the literature have been devoted to the derivation of continuous A- and L-stable collocation-based methods belonging to the family of two-step Runge-Kutta (TSRK) formulas introduced in [33, 34]. This is the case of two-step almost collocation (TSAC) methods, first derived in [21] and further analyzed in [20, 24, 25, 26, 33]. Similar methods for Volterra integral equations were investigated in [16, 17, 18] and for Volterra integro-differential equations in [13, 14]. Different approaches to the construction of continuous TSRK methods outside collocation have been presented in literature in the papers [3, 4, 35].

The nonlinear stability analysis of general linear methods (GLMs) for ODEs [12, 33] is subject of several recent papers, see for instance [11, 29, 30, 31, 32], where some classical results on algebraically stable Runge-Kutta methods [6, 7, 8, 9, 10, 11, 12, 19] have been extended to GLMs. Some preliminary results on the nonlinear stability properties of TSRK methods have been obtained in [22, 23], and examples of algebraically stable methods have been provided. It is the purpose of this work to analyze the nonlinear stability of two-step collocation methods of the form

$$\begin{cases} P(t_n + sh) = \varphi_0(s) y_{n-1} + \varphi_1(s) y_n + h \displaystyle\sum_{j=1}^{m} \Big(\chi_j(s) f(P(t_{n-1} + c_j h)) + \psi_j(s) f(P(t_n + c_j h)) \Big), \\ y_{n+1} = P(t_{n+1}), \end{cases} \tag{1.2}$$

where $t_n = t_0 + nh$, $n = 0, 1, \ldots, N$, $Nh = T - t_0$, is a uniform grid. The formulation of (1.2) is modelled by TSRK methods: in fact, advancing from the grid point t_n to the point t_{n+1}, the approximation y_{n+1} depends on the approximations y_{n-1} and y_n to the solution $y(t)$ of (1.1) at two consecutive step points t_{n-1} and t_n, and in addition on the stage

Email addresses: `dajconte@unisa.it` (Dajana Conte), `rdambrosio@unisa.it` (Raffaele D'Ambrosio), `jackiewi@math.la.asu.edu` (Zdzislaw Jackiewicz), `beapat@unisa.it` (Beatrice Paternoster)

derivatives related to the last two subintervals of integration. The continuous approximant $P(t_n+sh)$ is an algebraic polynomial which is obtained using a collocation approach described in [21]. This polynomial can be expressed as linear combination of the basis functions

$$\{\varphi_0(s),\ \varphi_1(s),\ \chi_j(s),\ \psi_j(s),\ j=1,2,\dots,m\},$$

which are unknown algebraic polynomials to be suitably determined. It is generally required that the polynomial $P(t_n+sh)$ satisfies the interpolation conditions

$$P(t_{n-1})=y_{n-1}, \quad P(t_n)=y_n, \tag{1.3}$$

and the collocation conditions

$$P'(t_{n-1}+c_jh)=f(P(t_{n-1}+c_jh)), \quad P'(t_n+c_jh)=f(P(t_n+c_jh)), \tag{1.4}$$

$j=1,2,\dots,m$. However, in order to obtain methods with strong stability properties such as, for example, A- or L-stability, we relax some of the interpolation and collocation conditions. This leads to additional free parameters which are then used to obtain methods with desirable stability properties. Following the terminology introduced in [21] the resulting methods are called TSAC methods. It is the main purpose of this paper to search for algebraically stable methods within this class of TSAC formulas.

The paper is organized as follows. In Section 2 we describe the family of TSAC methods introduced in [21] and recall their main properties. In Section 3 we provide the tools needed for the investigation of the algebraic stability properties of TSAC methods. Such tools are then employed in Section 4 in the search for algebraically stable TSAC methods, and examples of such formulas up to order $p=4$ are given. Finally, in Section 5 some concluding remarks are shown and future research plans are briefly outlined.

2. Two-step almost collocation methods

In the remainder of this paper we aim to analyze the nonlinear stability properties of TSAC methods (1.2). Such methods are obtained by fixing ρ basis functions among the set

$$\{\varphi_0(s),\ \chi_j(s),\ j=1,2,\dots,m\}, \tag{2.5}$$

as polynomials of degree $p=2m+1-\rho$, and deriving the remaining ones as solutions of the system of order conditions

$$\begin{cases} \varphi_0(s)+\varphi_1(s)=1, \\ \dfrac{(-1)^k}{k!}\varphi_0(s)+\displaystyle\sum_{j=1}^{m}\left(\chi_j(s)\frac{(c_j-1)^{k-1}}{(k-1)!}+\psi_j(s)\frac{c_j^{k-1}}{(k-1)!}\right)=\frac{s^k}{k!}, \end{cases} \tag{2.6}$$

$k=1,2,\dots,p$. Then, it was proved in [20, 21], that $p=2m+1-\rho$ is the uniform order of the resulting method.

The choice of ρ basis functions among the set (2.5) is made clear in Section 4, where the construction of algebraically stable TSAC methods (1.2) is described. Usually the ρ functions from the set (2.5) are also required to satisfy the conditions

$$\varphi_0(0)=0, \quad \chi_j(0)=0, \tag{2.7}$$

in order to guarantee that at least the interpolation condition $P(t_n)=y_n$ is satisfied. This follows as consequence of Theorem 2.4 in [21] which, in the hypothesis (2.7), ensures that

$$\varphi_1(0)=1, \quad \psi_j(0)=0.$$

The resulting collocation polynomial (1.2) is obtained as linear combination of the derived basis functions. In particular, we observe that by evaluating the collocation polynomial at $s=1$ and $s=c_i$, $i=1,2,\dots,m$, and by setting

$Y_i^{[n]} = P(t_n + c_i h)$, $i = 1,2,\dots,m$, TSAC methods (1.2) can be formulated as TSRK methods

$$\begin{cases} y_{n+1} = \theta y_{n-1} + \widetilde{\theta} y_n + h \sum_{i=1}^{m} \Big(v_i f(Y_i^{[n]}) + w_i f(Y_i^{[n-1]}) \Big), \\ Y_i^{[n]} = u_i y_{n-1} + \widetilde{u}_i y_n + h \sum_{j=1}^{m} \Big(a_{ij} f(Y_j^{[n]}) + b_{ij} f(Y_j^{[n-1]}) \Big), \end{cases} \tag{2.8}$$

where

$$\theta = \varphi_0(1), \quad \widetilde{\theta} = \varphi_1(1), \quad v_i = \psi_i(1), \quad w_i = \chi_i(1),$$
$$u_i = \varphi_0(c_i), \quad \widetilde{u}_i = \varphi_1(c_i), \quad a_{ij} = \psi_j(c_i), \quad b_{ij} = \chi_j(c_i),$$

$i, j = 1,2,\dots,m$. Observe that $\widetilde{\theta} = 1 - \theta$ and $\widetilde{u}_i = 1 - u_i$, $i = 1,2,\dots,m$. Moreover, we will next also use the formulation of TSAC methods as GLMs

$$\begin{cases} Y^{[n]} = h(\mathbf{A} \otimes \mathbf{I})F^{[n]} + (\mathbf{U} \otimes \mathbf{I})y^{[n]}, \\ y^{[n+1]} = h(\mathbf{B} \otimes \mathbf{I})F^{[n]} + (\mathbf{V} \otimes \mathbf{I})y^{[n]}, \end{cases} \tag{2.9}$$

where,

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_m^{[n]} \end{bmatrix}, \quad F^{[n]} = \begin{bmatrix} f(Y_1^{[n]}) \\ f(Y_2^{[n]}) \\ \vdots \\ f(Y_m^{[n]}) \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_n \\ y_{n-1} \\ hF^{[n-1]} \end{bmatrix},$$

and the matrices $\mathbf{A} \in \mathbb{R}^{m\times m}$, $\mathbf{U} \in \mathbb{R}^{m\times r}$, $\mathbf{B} \in \mathbb{R}^{r\times m}$, $\mathbf{V} \in \mathbb{R}^{r\times r}$, with $r = m+2$, assume the form

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

An interesting family of TSRK methods can be obtained choosing the parameter values $\theta = u_j = 0$, $j = 1,2,\dots,m$. With this choice, the corresponding TSRK methods can be represented as GLMs with input vector

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

and coefficient matrices $\mathbf{A}$, $\mathbf{U}$, $\mathbf{B}$ and $\mathbf{V}$ defined by

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

with $\mathbf{A} \in \mathbb{R}^{m\times m}$, $\mathbf{U} \in \mathbb{R}^{m\times r}$, $\mathbf{B} \in \mathbb{R}^{r\times m}$, $\mathbf{V} \in \mathbb{R}^{r\times r}$ and $r = m+1$. Observe that for the choice $\theta = 0$ and $u_i = 0$, $i = 1,2,\dots,m$, the dimensions of the matrices $\mathbf{U}$, $\mathbf{B}$, $\mathbf{V}$ are one less as compared with the general case $\theta \neq 0$ and $u_j \neq 0$, $j = 1,2,\dots,m$.

Remark 2.1. *Since $\theta = \varphi_0(1)$ and $u_i = \varphi_0(c_i)$, $i = 1,2,\dots,m$, TSAC methods equivalent to TSRK methods with $\theta = u_j = 0$, $j = 1,2,...,m$, are obtained choosing*

$$\varphi_0(s) = (s-1)\prod_{i=1}^{m}(s-c_i)\widetilde{\varphi}_0(s),$$

where $\widetilde{\varphi}_0(s)$ is an algebraic polynomial of degree $p-m-1$, if p is the order of the method. As a consequence, if the TSAC method has order $p = m$ or $p = m+1$ and satisfies the interpolation condition $\varphi_0(0) = 0$ in (2.7), then it necessarily follows that $\varphi_0(s) = 0$.

It was proved in [21] that the local discretization error of TSAC methods takes the form

$$\xi(t_{n+1}) = C_p(1)h^{p+1}y^{(p+1)}(t_n) + O(h^{p+2}), \tag{2.10}$$

where the continuous error constant $C_p(s)$, $s \in [0,1]$, is defined by

$$C_p(s) = \frac{s^{p+1}}{(p+1)!} - \frac{(-1)^{p+1}}{(p+1)!}\varphi_0(s) - \sum_{j=1}^{m}\left(\chi_j(s)\frac{(c_j-1)^p}{p!} + \psi_j(s)\frac{c_j^p}{p!}\right). \tag{2.11}$$

The quantity $h^{p+1}y^{(p+1)}(t_n)$ can be estimated by the expression having a similar form as the method itself. To be more precise it was proved in [21] that

$$h^{p+1}y^{(p+1)}(t_n) = \alpha_0 y_{n-1} + \alpha_1 y_n + h\sum_{j=1}^{m}\Big(\beta_j f(P(t_{n-1}+c_jh)) + \gamma_j f(P(t_n+c_jh))\Big) + O(h^{p+2}), \tag{2.12}$$

where the constants α_0, α_1, β_j, and γ_j, $j=1,2,\ldots,m$, satisfy the system of linear equations

$$\begin{cases} \alpha_0+\alpha_1 = 0, \\ \dfrac{(-1)^k}{k!}\alpha_0 + \displaystyle\sum_{j=1}^{m}\left(\beta_j\frac{(c_j-1)^{k-1}}{(k-1)!} + \gamma_j\frac{c_j^{k-1}}{(k-1)!}\right) = 0, \quad k=1,2,\ldots,p, \\ \left(\dfrac{(-1)^{p+1}}{(p+1)!} - C_p(-1)\right)\alpha_0 + \displaystyle\sum_{j=1}^{m}\left(\beta_j\frac{(c_j-1)^p}{p!} + \gamma_j\frac{c_j^p}{p!}\right) = 1. \end{cases} \tag{2.13}$$

Additional implementation issues for TSAC methods are investigated in a recent paper [25].

3. Search for algebraically stable TSAC methods

The representation of TSAC methods (1.2) as GLMs (2.9) allows us to exploit the recent results on the nonlinear stability properties of GLMs, which are formulated with respect to the nonlinear test problem

$$\begin{cases} y'(t) = g\big(t,y(t)\big), \quad t \geq 0, \\ y(0) = y_0, \end{cases} \tag{3.14}$$

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

$$\big(g(t,y_1) - g(t,y_2)\big)^T(y_1-y_2) \leq 0, \tag{3.15}$$

for all $t \geq 0$ and $y_1, y_2 \in \mathbb{R}^d$. Denote by $y(t)$ and $\widetilde{y}(t)$ two solutions to (3.14) with initial conditions y_0 and $\widetilde{y}_0$, respectively. Then the condition (3.15) implies that (3.14) is dissipative, i.e.,

$$\big\|y(t_2) - \widetilde{y}(t_2)\big\| \leq \big\|y(t_1) - \widetilde{y}(t_1)\big\|, \tag{3.16}$$

for $0 \leq t_1 \leq t_2$, compare [11, 27, 33].

Let $\{z^{[n]}\}_{n=0}^N$ be the solution to (2.9) with initial value $z^{[0]}$, and by $\{\widetilde{z}^{[n]}\}_{n=0}^N$ be the solution obtained by using a different initial value $\widetilde{z}^{[0]}$ or by perturbing the right hand side of (3.14). A GLM (2.9) is said to be G-stable if there exists a real, symmetric and positive definite matrix $\mathbf{G} \in \mathbb{R}^{r\times r}$ such that

$$\big\|z^{[n+1]} - \widetilde{z}^{[n+1]}\big\|_G \leq \big\|z^{[n]} - \widetilde{z}^{[n]}\big\|_G, \tag{3.17}$$

for all step sizes $h > 0$ and for all differential systems (3.14) with the function g satisfying (3.15), where

$$\|z\|_G^2 = \sum_{i=1}^{r}\sum_{j=1}^{r} g_{ij} z_i^T z_j, \qquad z_i \in \mathbb{R}^d,\ i=1,2,\ldots,r. \tag{3.18}$$

The GLM (2.9) 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 $\mathbf{D} \in \mathbb{R}^{m\times m}$ such that the matrix $\mathbf{M} \in \mathbb{R}^{(m+r)\times(m+r)}$ defined by

$$\mathbf{M} = \left[\begin{array}{c|c} \mathbf{DA}+\mathbf{A}^T\mathbf{D}-\mathbf{B}^T\mathbf{GB} & \mathbf{DU}-\mathbf{B}^T\mathbf{GV} \\ \hline \mathbf{U}^T\mathbf{D}-\mathbf{V}^T\mathbf{GB} & \mathbf{G}-\mathbf{V}^T\mathbf{GV} \end{array}\right] \tag{3.19}$$

is nonnegative definite. The significance of this definition follows from the result proved by Butcher [9, 10] (see also [28]), that for preconsistent and non-confluent GLMs (2.9), i.e. methods with distinct abscissas c_i, $i = 1,2,\dots,m$, algebraic stability is equivalent to *G*-stability.

It was observed by Hewitt and Hill [29, 30] that the verification if the matrix $\mathbf{M}$ is nonnegative definite can be simplified by the use of the following result proved by Albert [1].

Theorem 3.1. *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*

$$\mathbf{M}_{11} \geq 0, \quad \mathbf{M}_{22} - \mathbf{M}_{12}^T\mathbf{M}_{11}^+\mathbf{M}_{12} \geq 0, \quad \mathbf{M}_{11}\mathbf{M}_{11}^+\mathbf{M}_{12} = \mathbf{M}_{12}, \tag{3.20}$$

or, equivalently,

$$\mathbf{M}_{22} \geq 0, \quad \mathbf{M}_{11} - \mathbf{M}_{12}\mathbf{M}_{22}^+\mathbf{M}_{12}^T \geq 0, \quad \mathbf{M}_{22}\mathbf{M}_{22}^+\mathbf{M}_{12}^T = \mathbf{M}_{12}^T. \tag{3.21}$$

Here, $\mathbf{A}^+$ *stands for the Moore-Penrose pseudo-inverse of the matrix* $\mathbf{A}$*.*

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 large 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

$$\mathbf{N}(\xi) = \mathbf{A} + \mathbf{U}(\xi\mathbf{I}-\mathbf{V})^{-1}\mathbf{B}, \quad \xi \in \mathbb{C} - \sigma(\mathbf{V}), \tag{3.22}$$

where $\sigma(\mathbf{V})$ stands for the spectrum of the matrix $\mathbf{V}$. Denote by $\widetilde{\mathbf{w}}$ a principal left eigenvector of $\mathbf{V}$, i.e. the vector such that

$$\widetilde{\mathbf{w}}^T\mathbf{V} = \widetilde{\mathbf{w}}^T, \quad \widetilde{\mathbf{w}}^T\mathbf{q}_0 = 1, \tag{3.23}$$

where $\mathbf{q}_0$ is the preconsistency vector of GLMs (2.9). Following [31], we define the diagonal matrix $\widetilde{\mathbf{D}}$ by

$$\widetilde{\mathbf{D}} = \mathrm{diag}(\mathbf{B}^T\widetilde{\mathbf{w}}), \tag{3.24}$$

and by $\mathrm{He}(\mathbf{Q})$ the Hermitian part of a complex square matrix $\mathbf{Q}$, i.e.,

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

where $\mathbf{Q}^*$ stands for the conjugate transpose of $\mathbf{Q}$. We have the following result.

Theorem 3.2. *(compare [10, 31]). A consistent GLM (2.9) is algebraically stable if the following conditions are satisfied:*

1. *the coefficient matrix* $\mathbf{V}$ *is power-bounded;*
2. $\mathbf{Ux} \neq \mathbf{0}$ *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* $\widetilde{\mathbf{D}}\mathbf{A} \geq 0$*;*
4. $He\big(\widetilde{\mathbf{D}}\mathbf{N}(\xi)\big) \geq 0$ *for all* ξ *such that* $|\xi| = 1$ *and* $\xi \in \mathbb{C} - \sigma(\mathbf{V})$*.*

The numerical search for algebraically stable TSAC methods which is based on the criterion consisting of the conditions 1–4 in Theorem 3.2 is described in the Section 4.

We observe that, in the case of TSAC methods, 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 (3.23) is

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

and the matrix $\widetilde{\mathbf{D}}$ defined by (3.24) is

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

We next compute the Nyquist stability function $\mathbf{N}(\xi)$ corresponding to TSAC methods in the TSRK formulation (2.8) and the Hermitian part of $\widetilde{\mathbf{D}}\mathbf{N}(\xi)$. By using the inversion formula for block matrices (see [2]), we obtain

$$(\xi \mathbf{I} - \mathbf{V})^{-1} = \left[\begin{array}{cc|c} \dfrac{\xi}{\Delta} & \dfrac{\theta}{\Delta} & \dfrac{w^T}{\Delta} \\ \dfrac{1}{\Delta} & \dfrac{\xi - 1 + \theta}{\Delta} & \dfrac{w^T}{\xi \Delta} \\ \hline 0 & 0 & \dfrac{1}{\xi} I \end{array}\right],$$

where

$$\Delta = \xi(\xi - 1 + \theta) - \theta = (\xi - 1)(\xi + \theta).$$

This leads to

$$\begin{aligned} \mathbf{N}(\xi) &= \mathbf{A} + \mathbf{U}(\xi \mathbf{I} - \mathbf{V})^{-1}\mathbf{B} \\ &= A + \frac{\xi}{(\xi-1)(\xi+\theta)} e v^T + \frac{1}{(\xi-1)(\xi+\theta)} e w^T - \frac{1}{\xi+\theta} u v^T - \frac{1}{\xi(\xi+\theta)} u w^T + \frac{1}{\xi} B. \end{aligned}$$

We have also

$$\begin{aligned} \mathrm{He}\big(\widetilde{\mathbf{D}}\mathbf{N}(\xi)\big) = \frac{1}{2}\Bigg(& \widetilde{\mathbf{D}}\Big(A + \frac{1}{\xi}B\Big) + \Big(A^T + \frac{1}{\overline{\xi}}B^T\Big)\widetilde{\mathbf{D}} + \frac{\xi}{(\xi-1)(\xi+\theta)}\widetilde{\mathbf{D}} e v^T + \frac{\overline{\xi}}{(\overline{\xi}-1)(\overline{\xi}+\theta)} v e^T \widetilde{\mathbf{D}} - \frac{1}{\xi+\theta}\widetilde{\mathbf{D}} u v^T \\ & - \frac{1}{\overline{\xi}+\theta} v u^T \widetilde{\mathbf{D}} + \frac{1}{(\xi-1)(\xi+\theta)}\widetilde{\mathbf{D}} e w^T + \frac{1}{(\overline{\xi}-1)(\overline{\xi}+\theta)} w e^T \widetilde{\mathbf{D}} - \frac{1}{\xi(\xi+\theta)}\widetilde{\mathbf{D}} u w^T - \frac{1}{\overline{\xi}(\overline{\xi}+\theta)} w u^T \widetilde{\mathbf{D}} \Bigg). \end{aligned}$$

Using the relations

$$\begin{aligned} \widetilde{\mathbf{D}} e &= \frac{1}{1+\theta}(v+w), \quad e^T \widetilde{\mathbf{D}} = \frac{1}{1+\theta}(v+w)^T, \\ \widetilde{\mathbf{D}} u v^T &= \frac{1}{1+\theta}\big((v+w)\cdot u\big) v^T, \quad v u^T \widetilde{\mathbf{D}} = \frac{1}{1+\theta} v\big((v+w)\cdot u\big)^T, \\ \widetilde{\mathbf{D}} u w^T &= \frac{1}{1+\theta}\big((v+w)\cdot u\big) w^T, \quad w u^T \widetilde{\mathbf{D}} = \frac{1}{1+\theta} w\big((v+w)\cdot u\big)^T, \end{aligned}$$

where, $u \cdot v$ denotes componentwise multiplication of vectors, $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ can be written as

$$\begin{aligned}\mathrm{He}\big(\widetilde{\mathbf{D}}\mathbf{N}(\xi)\big) = \frac{1}{2(1+\theta)}\Bigg(&\mathrm{diag}(v+w)\Big(A+\frac{1}{\xi}B\Big)+\Big(A^T+\frac{1}{\overline{\xi}}B^T\Big)\mathrm{diag}(v+w)\\ &+\Big(\frac{\xi}{(\xi-1)(\xi+\theta)}+\frac{\overline{\xi}}{(\overline{\xi}-1)(\overline{\xi}+\theta)}\Big)vv^T+\Big(\frac{1}{(\xi-1)(\xi+\theta)}+\frac{\overline{\xi}}{(\overline{\xi}-1)(\overline{\xi}+\theta)}\Big)vw^T\\ &+\Big(\frac{\xi}{(\xi-1)(\xi+\theta)}+\frac{1}{(\overline{\xi}-1)(\overline{\xi}+\theta)}\Big)wv^T+\Big(\frac{1}{(\xi-1)(\xi+\theta)}+\frac{1}{(\overline{\xi}-1)(\overline{\xi}+\theta)}\Big)ww^T\\ &-\frac{1}{\xi+\theta}\big((v+w)\cdot u\big)v^T-\frac{1}{\overline{\xi}+\theta}v\big((v+w)\cdot u\big)^T-\frac{1}{\xi(\xi+\theta)}\big((v+w)\cdot u\big)w^T-\frac{1}{\overline{\xi}(\overline{\xi}+\theta)}w\big((v+w)\cdot u\big)^T\Bigg).\end{aligned}$$

With the aim of computing the limit

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

we observe that

$$\begin{aligned}\lim_{t\to 0}\Big(\frac{\xi}{(\xi-1)(\xi+\theta)}+\frac{\overline{\xi}}{(\overline{\xi}-1)(\overline{\xi}+\theta)}\Big)\Big|_{\xi=e^{it}} &= -\frac{1-\theta}{(1+\theta)^2},\\ \lim_{t\to 0}\Big(\frac{1}{(\xi-1)(\xi+\theta)}+\frac{\overline{\xi}}{(\overline{\xi}-1)(\overline{\xi}+\theta)}\Big)\Big|_{\xi=e^{it}} &= -\frac{2}{(1+\theta)^2},\\ \lim_{t\to 0}\Big(\frac{\xi}{(\xi-1)(\xi+\theta)}+\frac{1}{(\overline{\xi}-1)(\overline{\xi}+\theta)}\Big)\Big|_{\xi=e^{it}} &= -\frac{2}{(1+\theta)^2},\\ \lim_{t\to 0}\Big(\frac{1}{(\xi-1)(\xi+\theta)}+\frac{1}{(\overline{\xi}-1)(\overline{\xi}+\theta)}\Big)\Big|_{\xi=e^{it}} &= -\frac{3+\theta}{(1+\theta)^2}.\end{aligned}$$

The above discussion leads to the following result.

Theorem 3.3. *(compare [20, 23]) For a consistent TSAC method (1.2), the Hermitian part of the matrix* $\widetilde{\mathbf{D}}\mathbf{N}(\xi)$ *has the following limit*

$$\begin{aligned}\lim_{t\to 0}\mathrm{He}\big(\widetilde{\mathbf{D}}\mathbf{N}(\xi)\big)\Big|_{\xi=e^{it}} = \frac{1}{2(1+\theta)}\Bigg(&\mathit{diag}(v+w)\Big(A+B\Big)+(A+B)^T\mathit{diag}(v+w)-\frac{2}{(1+\theta)^2}(vw^T+wv^T)\\ &-\frac{1-\theta}{(1+\theta)^2}vv^T-\frac{3+\theta}{(1+\theta)^2}ww^T-\frac{1}{1+\theta}\Big(\big((v+w)\cdot u\big)(v+w)^T+(v+w)\big((v+w)\cdot u\big)^T\Big)\Bigg).\end{aligned} \tag{3.25}$$

Using this theorem we can make the search for algebraically stable GLMs more efficient by eliminating formulas for which the limit defined by (3.25) is less than zero.

An analogous result can be obtained in correspondence of the choice $\theta = 0$ and $u_i = 0$, $i = 1,2,\dots,m$. In this case, 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 (3.23) 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 (3.24) takes the form

$$\widetilde{\mathbf{D}} = \mathrm{diag}(v+w).$$

By means of arguments similar to that leading to Theorem 3.3, the hermitian part of the matrix $\widetilde{\mathbf{D}}N(\xi)$ behaves as follows

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

4. Derivation of algebraically stable TSAC methods

In this section we describe the derivation of algebraically stable TSAC methods with $m=1$, 2, 3, carried out by employing the tools provided in the previous section. In particular, in the case $m=1$, by applying Albert Theorem 3.1, we are able to determine classes of algebraically stable methods, together with their corresponding **G** and **D** matrices. In the case $m=2,3$, we have implemented an algorithm for the numerical search for algebraically stable TSAC methods written as GLMs (2.9). This algorithm is based on minimizing the objective function which computes the negative value of the minimum of the eigenvalues of the matrix

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi)), \quad \text{for } \xi \text{ such that } |\xi|=1 \text{ and } \ \xi\in\mathbb{C}\setminus\sigma(\mathbf{V}). \tag{4.26}$$

This objective function is a numerical realization of the necessary condition 4 for algebraic stability, which is listed in Theorem 3.2. Once the methods for which $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\geq 0$ for ξ such that $|\xi|=1$ and $\xi\in\mathbb{C}-\sigma(\mathbf{V})$ are found, the remaining necessary conditions 1-3 in Theorem 3.2 for algebraic stability are verified on the case by case basis.

Since A-stable TSAC methods with $m=1,2,3$ and $p>m+1$ have not been found in previous works (compare [20, 21]), we will describe next the search for algebraically stable methods with $p=m$ or $p=m+1$.

4.1. *Methods with $m=1$ and $p=2$*

We first consider the case of methods such that $\theta=u=0$. By relaxing the conditions on the basis function $\varphi_0(s)$, i.e., assuming that $\rho=1$, and imposing the interpolation condition $\varphi_0(0)=0$ we obtain, according to Remark 2.1, that $\varphi_0(s)=0$. By solving the system of order conditions (2.6) for $p=2$ we obtain

$$\varphi_1(s)=1, \quad \chi(s)=\frac{1}{2}s(2c-s), \quad \psi(s)=\frac{1}{2}s(2-2c+s).$$

In this way, a one-parameter family of TSAC methods depending on the collocation abscissa c arises. Such methods, according to the Schur criterion [36], are A-stable if and only if $c=1$. In this case, the stability polynomial is the same of the trapezoidal rule, which is A-stable, but not algebraically stable [28].

We next consider the case $\theta\neq 0$, $u\neq 0$, and relax the conditions on the basis function $\varphi_0(s)$ according to (2.7), by assuming

$$\varphi_0(s)=s(p_1+p_2s).$$

The order conditions (2.6) for $p=2$ lead to

$$\begin{aligned}\varphi_1(s) &= 1-p_1s-p_2s^2,\\ \chi_1(s) &= \tfrac{1}{2}s\left(p_1+(p_2-1)s+2c(p_1+p_2s+1)\right),\\ \psi_1(s) &= \tfrac{1}{2}s\left(p_1+p_2s+s-2c(p_1+p_2s+1)+2\right).\end{aligned}$$

In order to deal with a quadratic stability function (compare [15]), we assume that $p_1=-2cp_2$. In this way, a two-parameter family of TSAC methods arises, depending on p_2 and c. By applying the Schur criterion we obtain that such methods are A-stable if and only if

$$c>\frac{1}{2} \qquad \text{and} \qquad \frac{(c-1)^2}{c^2(2c-1)}<p_2<\frac{1}{2c-1}.$$

Assuming $c = 1$, $p_2 = 1/2$, and applying Albert conditions, we obtain an algebraically stable TSAC method for which the matrices $\mathbf{G}$ and $\mathbf{D}$ are defined by

$$\mathbf{G} = \begin{bmatrix} \frac{9}{10} & -\frac{19}{30} & -\frac{11}{30} \\ -\frac{19}{30} & \frac{1}{2} & \frac{3}{10} \\ -\frac{11}{30} & \frac{3}{10} & \frac{1}{5} \end{bmatrix}, \qquad \mathbf{D} = \begin{bmatrix} \frac{2}{15} \end{bmatrix}.$$

We obtain from (2.11) that the error constant associated to this method is $C_p(1) = 0$. Moreover, by solving the system (2.13), we can derive a one-parameter family of local error estimators of the type (2.12), with

$$\alpha_1 = -\alpha_0, \quad \beta_1 = \frac{3\alpha_0 - 2}{2}, \quad \gamma_1 = \frac{2 - \alpha_0}{2},$$

depending on the parameter α_0.

Another example of algebraically stable method corresponds to $c = 3/4$ and $p_2 = 3/2$. It can be verified using Theorem 3.1 that for this method the matrices $\mathbf{G}$ and $\mathbf{D}$ are defined by

$$\mathbf{G} = \begin{bmatrix} \frac{1987}{3750} & -\frac{641}{1250} & -\frac{1769}{3750} \\ -\frac{641}{1250} & \frac{1}{2} & \frac{23}{50} \\ -\frac{1769}{3750} & \frac{23}{50} & \frac{127}{300} \end{bmatrix}, \qquad \mathbf{D} = \begin{bmatrix} \frac{8}{1875} \end{bmatrix}.$$

In this case, we have $C_p(1) = 0$ and, by solving the system (2.13), a one-parameter family of local error estimators (2.12) arises, with

$$\alpha_1 = -\alpha_0, \quad \beta_1 = \frac{5\alpha_0 - 4}{4}, \quad \gamma_1 = \frac{4 - \alpha_0}{4},$$

depending on the parameter α_0.

4.2. Methods with $m = p = 1$

We first consider the case of methods such that $\theta = u = 0$. We relax the conditions on $\rho = 2$ basis functions and impose the conditions (2.7) which take now the form

$$\varphi_0(0) = 0, \quad \chi(0) = 0.$$

As a consequence of these choices, and taking into account Remark 2.1, we obtain

$$\varphi_0(s) = 0, \quad \chi(s) = r_1 s. \tag{4.27}$$

We determine the other basis functions by solving the system of order conditions (2.6) for $p = 1$, which leads to

$$\varphi_1(s) = 1, \quad \psi(s) = (1 - r_1)s.$$

We analyze the A-stability properties of the resulting methods by using the Schur criterion: each method belonging to the derived two-parameter family of methods is A-stable if and only if

$$\left(r_1 \leq 0 \quad \text{and} \quad c > \frac{1}{2} \right) \quad \text{or} \quad \left(0 < r_1 < \frac{1}{2} \quad \text{and} \quad c > \frac{1}{2}(1 + r_1) \right).$$

Moreover, the following result holds.

Theorem 4.1. *A-stable TSAC methods with $m = p = 1$ and basis functions (4.27) are also algebraically stable, with*

$$\mathbf{G} = \begin{bmatrix} 1 & r_1 \\ r_1 & r_1^2 - c r_1 + c - \frac{1}{2} \end{bmatrix}, \qquad \mathbf{D} = [1] \tag{4.28}$$

Proof: For the matrices **G** and **D** defined in (4.28), the matrix **M** in (3.19) takes the form

$$\mathbf{M} = \begin{bmatrix} -r_1 c + c - \frac{1}{2} & 0 & (c-1)r_1 \\ 0 & 0 & 0 \\ (c-1)r_1 & 0 & -r_1 c + c - \frac{1}{2} \end{bmatrix}.$$

Theorem 3.1 ensures that this matrix is nonnegative definite, which concludes the proof. □

We next consider the case $\theta \neq 0$, $u \neq 0$. Following [24] we assume that

$$\varphi_0(s) = p_1 s, \quad \chi(s) = q_1 s, \tag{4.29}$$

and derive the remaining basis functions by imposing the order conditions. In this way, a three-parameter family of methods arises, depending on the values of the parameters p_1, q_1 and c. The A-stability properties of such methods have been analyzed in [24], by means of the Schur criterion (see Fig. 1).

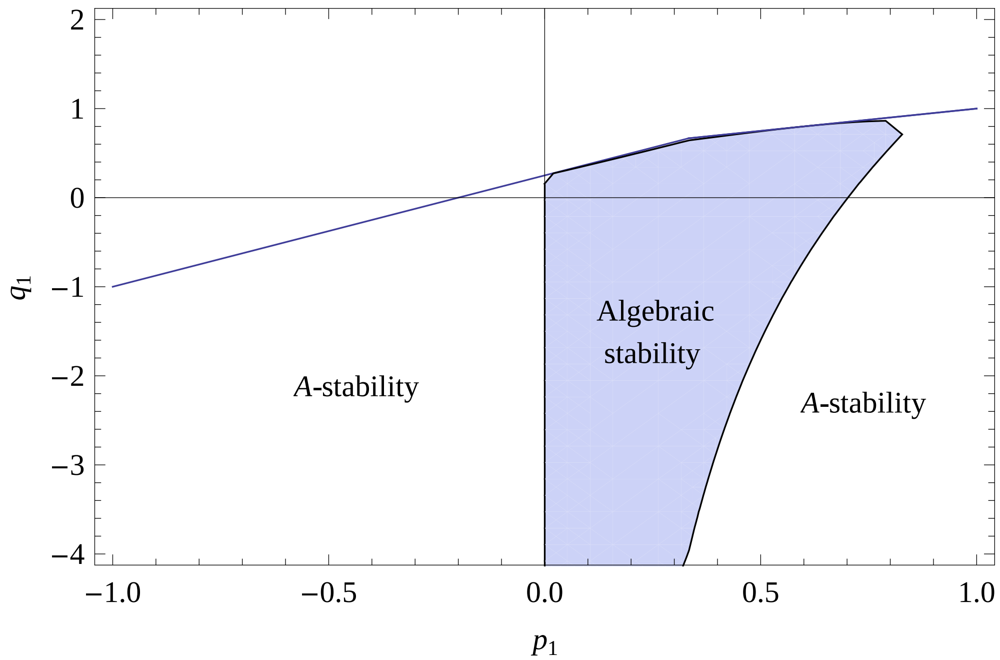

Figure 1: Region of A- and algebraic stability in the (p_1, q_1)-plane of TSAC methods (1.2) with $m = p = 1$, basis functions (4.29), $c = 3/4$ and α given by (4.33)

Sufficient conditions for algebraically stable TSAC methods are given by the following result.

Theorem 4.2. *TSAC methods (1.2) with $m = p = 1$ and basis functions (4.29) are algebraically stable if the parameters p_1, q_1 and c satisfy the conditions*

$$\begin{cases} 0 < p_1 < 1, \\ -\alpha^2(p_1-1)^2 p_1^2 - (cp_1 + c - 1)^2 (p_1 - q_1)^2 \\ \qquad + \alpha(p_1-1)p_1\left(c^2 p_1 (p_1+1)^2 + 2c\left(p_1\left(p_1^2 - p_1 q_1 - 2\right) + q_1 - 1\right)\right. \\ \qquad \left. + p_1\left(-2p_1 q_1 + (p_1-1)p_1 + q_1^2 + 1\right) + 1\right) \geq 0, \end{cases} \tag{4.30}$$

where $\alpha > 0$ is a fixed parameter.

Proof: Define the matrices **G** and **D** by

$$\mathbf{G} = \begin{bmatrix} \dfrac{1}{p_1} & 0 & -\dfrac{p_1-q_1}{p_1} \\ 0 & 1 & 1 \\ -\dfrac{p_1-q_1}{p_1} & 1 & \dfrac{2p_1q_1-p_1-q_1^2}{p_1^2-p_1}+\alpha \end{bmatrix}, \tag{4.31}$$

and

$$\mathbf{D} = \begin{bmatrix} \dfrac{1+p_1}{p_1} \end{bmatrix}. \tag{4.32}$$

The first hypothesis in (4.30) and the condition $\alpha > 0$ ensure that **G** and **D** are positive definite. The corresponding matrix **M** defined by (3.19) assumes the form

$$\mathbf{M} = \begin{bmatrix} m_{11} & -p_1c-c+1 & p_1c+c-1 & \dfrac{(p_1c+c-1)q_1}{p_1} \\ -p_1c-c+1 & 1-p_1 & p_1-1 & q_1-1 \\ p_1c+c-1 & p_1-1 & 1-p_1 & 1-q_1 \\ \dfrac{(p_1c+c-1)q_1}{p_1} & q_1-1 & 1-q_1 & \dfrac{\alpha(p_1-1)-(q_1-1)^2}{p_1-1} \end{bmatrix},$$

where

$$m_{11} = \frac{p_1\left((p_1-q_1)^2+\alpha-\alpha p_1-p_1\right)+2c\left(p_1^2-1\right)(p_1-q_1+1)+1}{(p_1-1)p_1}.$$

By applying the Albert Theorem 3.1 and employing the second hypothesis in (4.30), it follows that the matrix **M** is nonnegative definite. This completes the proof. □

In Fig. 1 the region of *A*- and algebraic stability in the (p_1, q_1)-plane is reported for $c = 3/4$ and

$$\alpha = \frac{49p_1^3-56p_1^2q_1+2p_1^2+16p_1q_1^2-23p_1+24q_1-8}{32(p_1-1)p_1}, \tag{4.33}$$

inside the *A*-stability region. In particular, by making the choice $p_1 = q_1$, Theorem 4.2 allows to find algebraically stable formulae for any value of the abscissa c greater than $1/2$. This situation is described in the following result.

Corollary 4.1. *TSAC methods (1.2) with $m = p = 1$ and basis functions (4.29) with $p_1 = q_1$ are algebraically stable for any choice of the parameters p_1 and c within the region $\mathscr{A} \cup \mathscr{B}$, where $\mathscr{A}$ and $\mathscr{B}$ are the regions given by*

$$\mathscr{A} = \left\{(c, p_1):\ \frac{1}{2} < c \le \beta \quad \text{and} \quad \left(0 < p_1 < \gamma_1(c) \quad \text{or} \quad \gamma_2(c) < p_1 < \gamma_3(c)\right)\right\},$$

$$\mathscr{B} = \left\{(c, p_1):\ c > \beta \quad \text{and} \quad 0 < p_1 < \gamma_1(c)\right\}.$$

Here, β is the positive root of the polynomial

$$4x^3+32x^2-8x-5,$$

and $\gamma_1(c)$, $\gamma_2(c)$ and $\gamma_3(c)$ are the roots of the polynomial

$$c^2x^3+(2c^2-1)x^2+(c^2-2c+1)x+1-2c.$$

Proof: The second condition in (4.30) of Theorem 4.2 for $p_1 = q_1$ reduces to

$$-(\alpha+1)(p_1-1)p_1 + c^2 p_1(p_1+1)^2 - 2c(p_1+1) + 1 \le 0,$$

whose left hand side identically vanishes by choosing

$$\alpha = \frac{1 + p_1 - p_1^2 - 2c(1+p_1) + c^2 p_1 (1+p_1)^2}{p_1(p_1-1)}.$$

Then, the algebraic stability conditions of Theorem 4.2 reduce to $0 < p_1 < 1$ and $\alpha > 0$, which are satisfied for any $(c, p_1) \in \mathscr{A} \cup \mathscr{B}$. It can be verified that the matrices $\mathbf{G}$ and $\mathbf{D}$ associated with these algebraically stable methods are given by

$$\mathbf{G} = \begin{bmatrix} \dfrac{1}{p_1} & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1+\alpha \end{bmatrix}, \quad \mathbf{D} = \begin{bmatrix} \dfrac{1+p_1}{p_1} \end{bmatrix}.$$

□

Observe that the condition $c > 1/2$, together with the condition for zero-stability $0 < p_1 < 1$, is a necessary condition to achieve A-stability. In fact, by applying the Schur criterion to the methods of Corollary 4.1, the region of A-stability in the parameter space (c, p_1) is $(1/2, \infty) \times (0, 1)$. Fig. 2 shows the algebraic stability region $\mathscr{A} \cup \mathscr{B}$ inside the A-stability one, in the rectangle $(1/2, 1) \times (-1, 1)$.

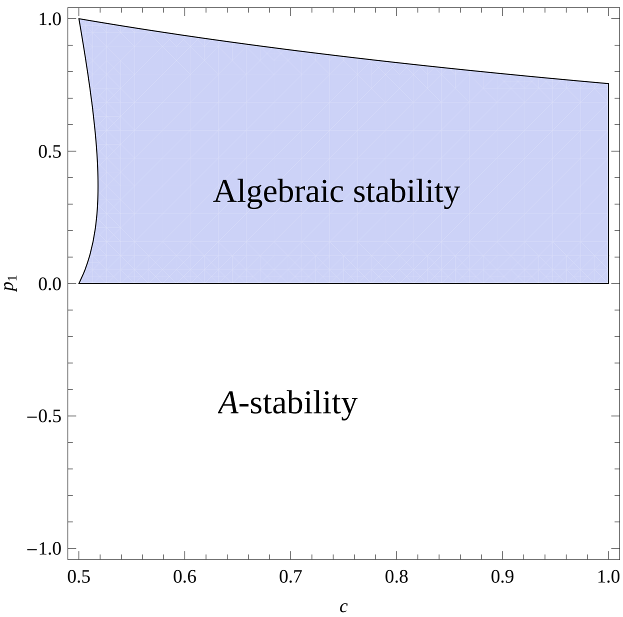

Figure 2: Region of $A-$ and algebraic stability in the (c, p_1)-plane for TSAC methods (1.2) of Corollary 4.1

Finally, we have searched for $L-$stable methods which are also algebraically stable. It has been proved in [24] that TSAC methods with $m = p = 1$ and basis functions (4.29) are L-stable if $c = 1$, $q_1 = 0$ and $p_1 \in (-1, 1]$. By using Theorem 4.2 with the parameter α given by

$$\alpha = \frac{-1 - 2p_1 + p_1^2 + 4p_1^3}{2(p_1-1)p_1},$$

we obtain L- and algebraically stable methods for the parameter values $c = 1$, $q_1 = 0$, and $p_1 \in (0, (1+\sqrt{17})/8)$.

4.3. Methods with $m = 2$ and $p = 3$

Our search for algebraically stable methods with $m = 2$ and $p = 3$ will be carried out inside the class of A-stable methods derived in [21]. Therefore, following [21], we impose the interpolation conditions (2.7) which take the form

$$\varphi_0(0) = 0, \quad \chi_1(0) = 0,$$

and we fix the $\rho = 2$ basis functions

$$\varphi_0(s) = s\left(q_2 s^2 + q_1 s + q_0\right), \quad \chi_1(s) = s\left(r_2 s^2 + r_1 s + r_0\right),$$

where q_2, q_1, q_0, r_2, r_1, and r_0 are real parameters. We next derive the values of these parameters realizing the collocation conditions

$$\varphi_0'(c_1) = \varphi_0'(c_2) = 0 \quad \text{and} \quad \chi_1'(c_1) = \chi_1'(c_2) = 0.$$

This leads to

$$q_1 = -\frac{(c_1 + c_2)q_0}{2c_1c_2}, \quad q_2 = \frac{q_0}{3c_1c_2}, \quad r_1 = -\frac{(c_1 + c_2)r_0}{2c_1c_2}, \quad r_2 = \frac{r_0}{3c_1c_2}.$$

We next determine the remaining basis functions $\varphi_1(s)$, $\chi_2(s)$, $\psi_1(s)$, and $\psi_2(s)$ by imposing the system of order conditions for $p = 3$. As in [21], we fix $c_1 = 5/2$ and $c_2 = 9/2$. This leads to a two-parameter family of TSAC methods, depending on q_0 and r_0. Within this family, we search for algebraically stable methods, by minimizing the negative value of the objective function computing the minimum of the eigenvalues of the matrix (4.26). For instance, for

$$q_0 = -0.4253608181543406, \quad r_0 = 1.6033382155047602, \tag{4.34}$$

we obtain a method satisfying

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq 0, \quad t \in [0, 2\pi].$$

This bound has been obtained by dividing the interval $[0, 2\pi]$ into $n = 10000$ subintervals. The eigenvalues of $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ for $\xi = e^{it}$, $t \in [0, 2\pi]$, are plotted in Fig. 3.

4.4. Methods with $m = 2$ and $p = 2$

Our search for algebraically stable methods with $m = 2$ and $p = 2$ will be carried out inside the class of A-stable methods derived in [25]. Therefore, following [25], we impose the interpolation conditions (2.7) which are given by

$$\varphi_0(0) = \chi_1(0) = \chi_2(0) = 0,$$

and assume that $\varphi_0(s)$, $\chi_1(s)$, and $\chi_2(s)$ take the form

$$\varphi_0(s) = s(p_1 + p_2 s), \quad \chi_1(s) = s(q_1 + q_2 s), \quad \chi_2(s) = s(r_1 + r_2 s),$$

where p_1, p_2, q_1, q_2, r_1, and r_2 are real parameters. Then solving the system of order conditions for $p = 2$ we obtain a six-parameter family of methods of order $p = 2$ depending on these parameters. Next, we looked for algebraically stable methods within the class of A- and L-stable TSAC methods derived in [25] for $c_1 = 1/2$, $c_2 = 1$, and

$$p_1 = -\frac{2p_2(1 + r_2)}{2 + r_2}, \quad q_1 = \frac{2p_1}{p_2}, \quad r_1 = -\frac{2r_2(1 + r_2)}{2 + r_2}, \quad q_2 = 2.$$

Fig. 4 shows the region of $A-$ and $L-$ stability in the parameter space (p_2, r_2). Corresponding to the asterisks marked in Fig. 4, we found formulas for which

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq -10^{-9}, \quad t \in [0, 2\pi]. \tag{4.35}$$

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, this bound is equal to 0. The circled asterisk in Fig. 4 corresponds to the values

$$p_2 = 0.7567262495625600, \quad r_2 = -0.4460521573543530, \tag{4.36}$$

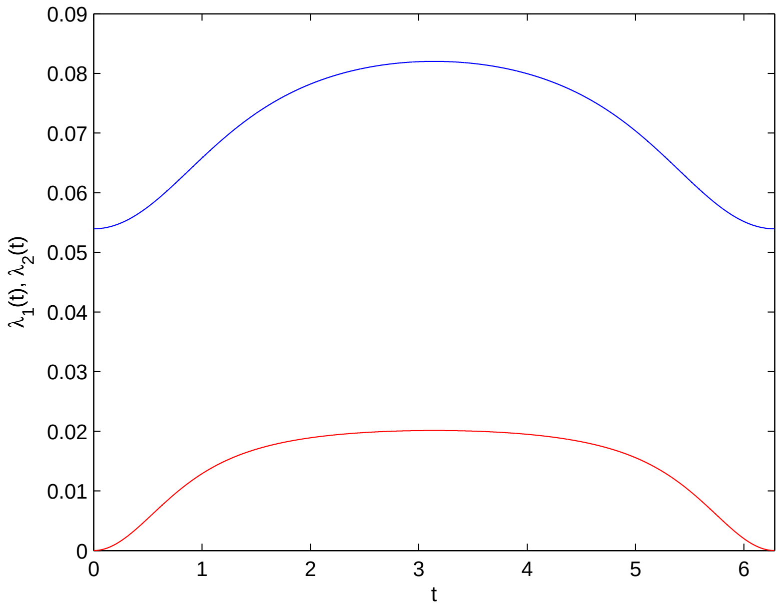

Figure 3: Eigenvalues $\lambda_1(t)$ and $\lambda_2(t)$ of the matrix $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ for $\xi = e^{it}$, $t \in [0,2\pi]$, in correspondence to the choices (4.34) of the free parameters q_0 and r_0

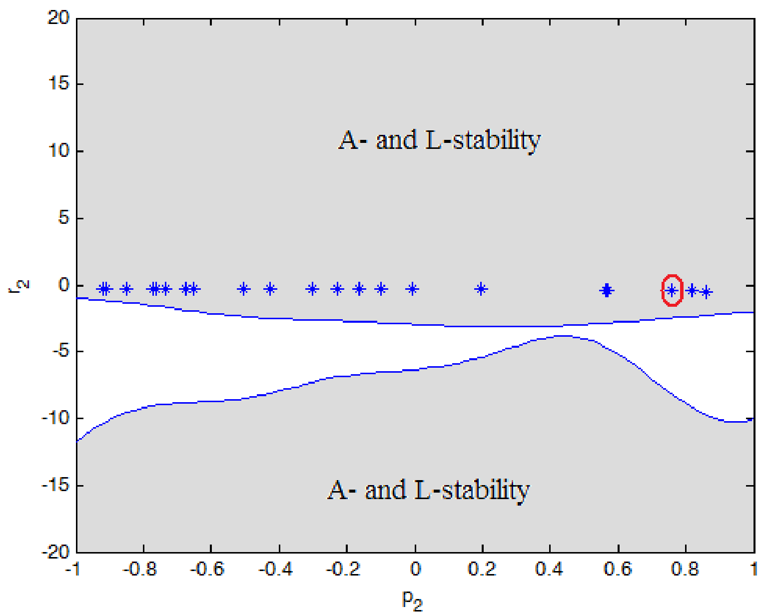

Figure 4: Region of A- and L- stability in the parameter space (p_2, r_2). $*$: methods satisfying the bound (4.35). $\circledast$: method satisfying the bound (4.37)

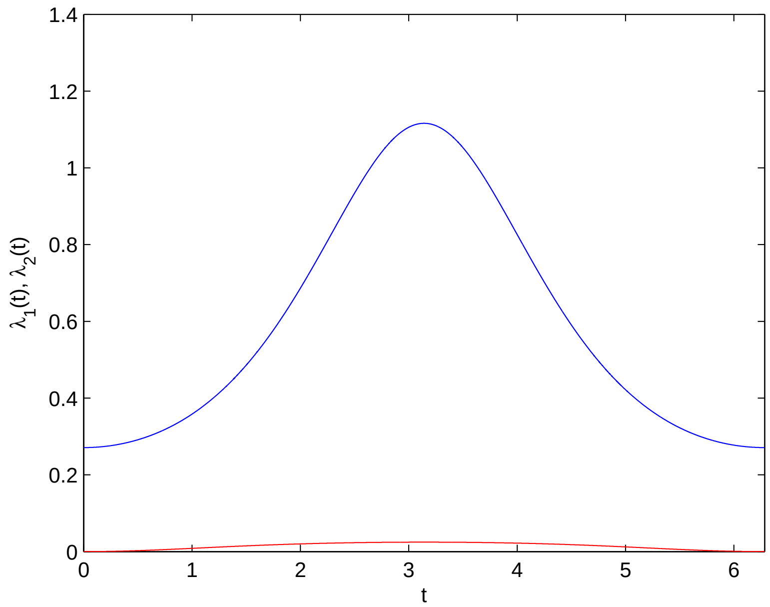

Figure 5: Eigenvalues $\lambda_1(t)$ and $\lambda_2(t)$ of the matrix $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ for $\xi = e^{it}$, $t \in [0,2\pi]$, in correspondence to the choices (4.36) of the free parameters p_2 and r_2

and the resulting method is L-stable and satisfies the bound

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq 0, \quad t \in [0,2\pi]. \tag{4.37}$$

This bound has been obtained by dividing the interval $[0,2\pi]$ into $n = 10000$ subintervals. The eigenvalues of $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ for $\xi = e^{it}$, $t \in [0,2\pi]$, are plotted in Fig. 5.

We obtain from (2.11) that the error constant associated to this method is

$$C_p(1) = -0.18492969764966272.$$

Moreover, by solving the system (2.13), we can derive a two-parameter family of local error estimators of the type (2.12), with

$$\alpha_1 = -\alpha_0, \quad \beta_1 = 4 - 7.408910647463099\alpha_0 - \gamma_2,$$
$$\beta_2 = -8 + 16.817821294926198\alpha_0 + 3\gamma_2, \quad \gamma_1 = 4 - 8.408910647463099\alpha_0 - 3\gamma_2,$$

depending on the parameters α_0 and γ_2.

4.5. Methods with $m = 3$ and $p = 4$

In this case, we relax the following $\rho = 3$ basis functions

$$\varphi_0(s) = s\left(\sum_{i=1}^{3} \ell_i(s)\frac{r_i}{c_i} + \ell_4(s)r_4\right), \quad \chi_1(s) = s\left(\sum_{i=1}^{3} \ell_i(s)\frac{q_i}{c_i} + \ell_4(s)q_4\right), \quad \chi_2(s) = s\left(\sum_{i=1}^{3} \ell_i(s)\frac{s_i}{c_i} + \ell_4(s)s_4\right). \tag{4.38}$$

These functions satisfy the interpolation conditions (2.7), where $\ell_i(s)$, $i = 1,2,3,4$, are the Lagrange fundamental polynomials associated to the abscissas $\{c_1, c_2, c_3, 1\}$. We next derive the remaining basis functions by imposing the

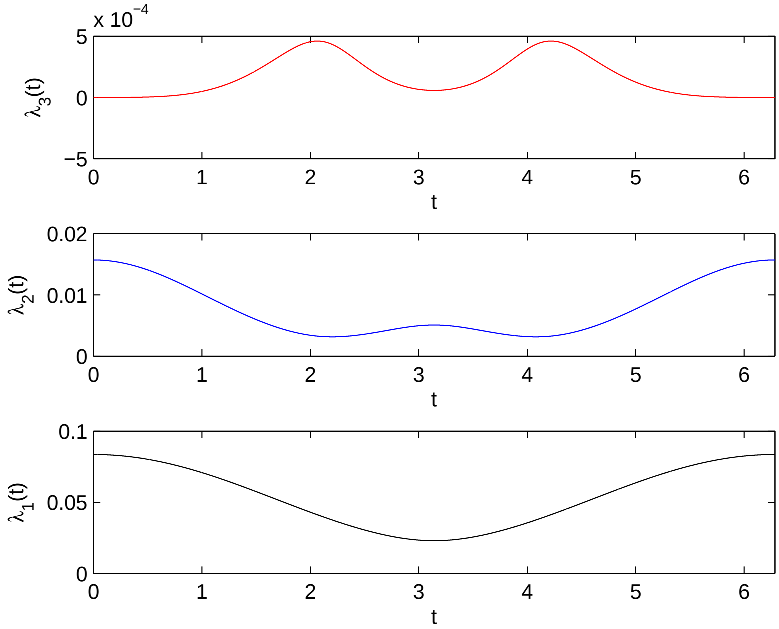

Figure 6: Eigenvalues $\lambda_1(t)$, $\lambda_2(t)$ and $\lambda_3(t)$ of the matrix $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ for $\xi = e^{it}$, $t \in [0, 2\pi]$

system of order conditions up to order $p = 4$. In this way, we obtain a 15-parameter family of TSAC methods (1.2), depending on c_j, $j = 1,2,3$ and q_i, r_i, s_i, $i = 1,2,3,4$, which represent the evaluations of the basis functions (4.38) in $\{c_1, c_2, c_3, 1\}$, i.e.

$$\begin{array}{llll} \chi_1(c_1) = q_1, & \chi_1(c_2) = q_2, & \chi_1(c_3) = q_3, & \chi_1(1) = q_4, \\ \chi_2(c_1) = s_1, & \chi_2(c_2) = s_2, & \chi_2(c_3) = s_3, & \chi_2(1) = s_4, \\ \varphi_0(c_1) = r_1, & \varphi_0(c_2) = r_2, & \varphi_0(c_3) = r_3, & \varphi_0(1) = r_4. \end{array}$$

We carry out a numerical search for algebraically stable methods and for the parameters

$$\begin{array}{ll} q_1 = -0.2726789592434525, & q_2 = -0.4181859079468002, \\ q_3 = -0.4081521541939172, & q_4 = -0.3900512337727580, \\ r_1 = 0.0254105370486458, & r_2 = -0.0410914281399805, \\ r_3 = -0.0865247300437837, & r_4 = -0.0406851876697910, \\ s_1 = -0.0345953002848433, & s_2 = -0.0027633289164017, \\ s_3 = -0.1546470396551506, & s_4 = -0.0293367577248120, \\ c_1 = 0.8052565472589601, & c_2 = 0.2883202630501468, \\ c_3 = -0.2961982211404683, & \end{array}$$

we obtain a method satisfying

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq 0, \quad t \in [0, 2\pi].$$

This bound has been obtained by dividing the interval $[0, 2\pi]$ into $n = 10000$ subintervals. The eigenvalues of $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ for $\xi = e^{it}$, $t \in [0, 2\pi]$, are plotted in Fig. 6.

We obtain from (2.11) that the error constant associated to this method is

$$C_p(1) = 0.13146585625709778.$$

Moreover, by solving the system (2.13), we derive a two-parameter family of local error estimators of the type (2.12), with

$$\alpha_0 = -0.16308569769132666, \quad \alpha_1 = 0.16308569769132666,$$
$$\beta_1 = -0.07010794285202898 - 1.4385688179398948\gamma_2 - 0.803738349389213\gamma_3,$$
$$\beta_2 = -0.0887295271619641 + 0.8632491086735037\gamma_2 - 0.24380158546810216\gamma_3,$$
$$\beta_3 = -0.0038847814923057837 - 0.1845680275203434\gamma_2 + 0.034316728210577824\gamma_3,$$
$$\gamma_1 = -0.0003634461850278035 - 0.240112263213288\gamma_2 + 0.013223206646738105\gamma_3,$$

depending on the parameters γ_2 and γ_3.

4.6. Methods with $m = 3$ and $p = 3$

In this case, we relax the $\rho = 4$ basis functions

$$\varphi_0(s) = \sum_{i=1}^{4} \ell_i(s) r_i, \quad \chi_1(s) = \sum_{i=1}^{4} \ell_i(s) q_i, \quad \chi_2(s) = \sum_{i=1}^{4} \ell_i(s) s_i, \quad \chi_3(s) = \sum_{i=1}^{4} \ell_i(s) p_i,$$

where $\ell_i(s)$, $i = 1,2,3,4$, are the fundamental Lagrange polynomials associated to the abscissas $\{c_1, c_2, c_3, 1\}$. We next derive the remaining basis functions by imposing the system of order conditions up to order $p = 3$. This leads to a 19-parameter family of TSAC methods depending on c_j, $j = 1,2,3$ and q_i, r_i, s_i, p_i, $i = 1,2,3,4$, which represent the evaluations of the basis functions (4.38) in $\{c_1, c_2, c_3, 1\}$, i.e.

$$\begin{array}{llll}
\chi_1(c_1) = q_1, & \chi_1(c_2) = q_2, & \chi_1(c_3) = q_3, & \chi_1(1) = q_4, \\
\chi_2(c_1) = s_1, & \chi_2(c_2) = s_2, & \chi_2(c_3) = s_3, & \chi_2(1) = s_4, \\
\chi_3(c_1) = p_1, & \chi_3(c_2) = p_2, & \chi_3(c_3) = p_3, & \chi_3(1) = p_4, \\
\varphi_0(c_1) = r_1, & \varphi_0(c_2) = r_2, & \varphi_0(c_3) = r_3, & \varphi_0(1) = r_4.
\end{array}$$

We carry out a numerical search for algebraically stable methods and for

$$\begin{array}{ll}
p_1 = 0.2161653206100524, & p_2 = 0.5305046665091202, \\
p_3 = 0.5006036194861265, & p_4 = -0.0442411660931498, \\
q_1 = 0.4890828798433550, & q_2 = -0.0436404150461699, \\
q_3 = 0.4863106562462140, & q_4 = 0.2325277079503709, \\
r_1 = 0.0578387262996022, & r_2 = -0.2486414601865061, \\
r_3 = 0.4182238288736025, & r_4 = -0.1101403829440502, \\
s_1 = -0.6730527554702595, & s_2 = 0.9200313313645769, \\
s_3 = -1.4427135243568587, & s_4 = -0.0472056454517496, \\
c_1 = 1.6279435207726001, & c_2 = 0.7466367275877779, \\
c_3 = 0.2657929207108657, &
\end{array}$$

we obtain a method satisfying

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi = e^{it}} \geq 0, \quad t \in [0, 2\pi].$$

This bound has been obtained by dividing the interval $[0, 2\pi]$ into $n = 10000$ subintervals. The eigenvalues of $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ for $\xi = e^{it}$, $t \in [0, 2\pi]$, are plotted in Fig. 7.

In this case, we obtain from (2.11) that the error constant associated to this method is

$$C_p(1) = 0.0035029427463059287.$$

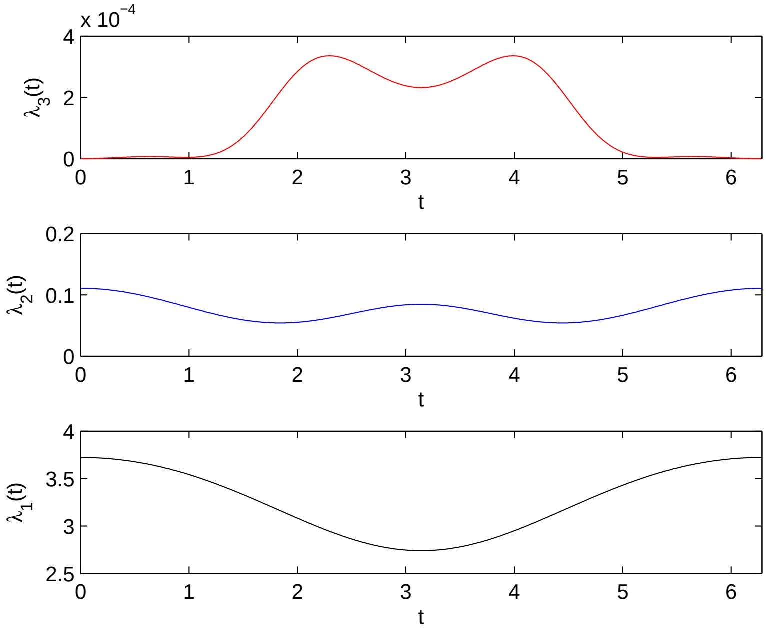

Figure 7: Eigenvalues $\lambda_1(t)$, $\lambda_2(t)$ and $\lambda_3(t)$ of the matrix $\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))$ for $\xi = e^{it}$, $t \in [0, 2\pi]$

Moreover, by solving the system (2.13), we derive a three-parameter family of local error estimators of the type (2.12), with

$$\alpha_0 = -0.027309616275544915 + 0.020227003707928848\gamma_1 + 0.0008000174585913733\gamma_2 - 0.0008557592376018386\gamma_3,$$
$$\alpha_1 = 0.027309616275544915 - 0.020227003707928848\gamma_1 - 0.0008000174585913733\gamma_2 + 0.0008557592376018386\gamma_3,$$
$$\beta_1 = -0.0005816766234610915 - 3.701386325079529\gamma_1 - 1.2335336759648714\gamma_2 - 0.43247807915787195\gamma_3,$$
$$\beta_2 = -0.011654042794290243 + 5.5827532200160395\gamma_1 + 0.4151081846801168\gamma_2 - 0.8549556923760194\gamma_3,$$
$$\beta_3 = -0.015073896857793579 - 2.8611398912285817\gamma_1 - 0.18077449125665404\gamma_2 + 0.2865780122962896\gamma_3,$$

depending on the parameters γ_1, γ_2 and γ_3.

5. Conclusions and future work

We have presented the approaches for systematic search for algebraically stable GLMs for ODEs, based on Albert theorem and the recent criteria formulated by Hill, which are based on Nyquist stability function. These searches were illustrated on TSAC methods up to uniform order $p = 4$. Future work will address the construction of algebraically stable TSAC methods of high order and the derivation of the **G**-matrices (for instance according to [32]) of the derived methods.

Future work will also address various implementations issues related to these methods and comparison with classical methods for ODEs such as Runge-Kutta and linear multistep methods. The realization of this program requires the derivation of efficient local error estimators for small and large stepsizes, the design of stepsize and order changing strategies and efficient solution of nonlinear systems of equations by some variants of Newton method at each step of integration. The techniques to accomplish these goals are different from those employed in this note and these topics will be the subject of separate paper.

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