Two-step Runge-Kutta methods with quadratic stability functions

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Abstract. We describe the construction of implicit two-step Runge-Kutta methods with stability properties determined by quadratic stability functions. We will aim for methods which are A-stable and L-stable and such that the coefficients matrix has a one point spectrum. Examples of methods of order up to eight are provided.

Keywords: Two-step Runge-Kutta methods, order conditions, quadratic stability polynomials, absolute stability, A-stability, L-stability.

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1 Introduction

For the numerical solution of initial-value problems for ordinary differential equations (ODEs)

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

$f : \mathbb{R}^m \to \mathbb{R}^m$, we consider the class of two-step Runge-Kutta (TSRK) methods of the form

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

$i = 1, 2, \ldots, s$, $n = 2, 3, \ldots, N$, $Nh = T - t_0$. Here, y_n is an approximation of order p to $y(t_n)$, $t_n = t_0 + nh$, and $Y_i^{[n]}$ are approximations of stage order q to $y(t_{n-1} + c_i h)$, $i = 1, 2, \ldots, s$, where $y(t)$ is the solution to (1.1), $c = [c_1, \ldots, c_s]^T$ is the abscissa vector and $-1 < \theta \le 1$ for zero-stability. The precise definitions of order and stage order are given in Section 2. These methods were introduced by Jackiewicz and Tracogna [24] and further investigated in [1], [2], [3], [4], [13], [17], [21], [25], [26], [29], and [30].

TSRK methods (1.2) can be represented by the abscissa vector c and the table of their coefficients

$$\begin{array}{c|c|c} u & A & B \\ \hline \theta & v^T & w^T \end{array} = \begin{array}{c|cccc|cccc} u_1 & a_{11} & a_{12} & \cdots & a_{1s} & b_{11} & b_{12} & \cdots & b_{1s} \\ u_2 & a_{21} & a_{22} & \cdots & a_{2s} & b_{21} & b_{22} & \cdots & b_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ u_s & a_{s1} & a_{s2} & \cdots & a_{ss} & b_{s1} & b_{s2} & \cdots & b_{ss} \\ \hline \theta & v_1 & v_2 & \cdots & v_s & w_1 & \cdots & w_{s-1} & w_s \end{array}.$$

In this paper we will describe a new approach for the construction of methods of order p and stage order $q = p$ for which stability properties are determined by quadratic stability functions. Since $p = q$ these methods do not suffer from order reduction phenomenon which is the case for classical Runge-Kutta methods. This is illustrated numerically in Section 8. Moreover, we assume that the coefficient matrix B has a one point spectrum

$$\sigma(B) = \{\lambda\}, \quad \lambda > 0. \tag{1.3}$$

This feature would allow for efficient implementation of such methods similarly as in the case of singly implicit Runge-Kutta (SIRK) methods considered by Burrage [6], Butcher [8], and Burrage, Butcher and Chipman [7], see also [9], [11].

Putting $Y^{[n]} = [Y_1^{[n]}, \ldots, Y_s^{[n]}]^T$, $f(Y^{[n]}) = [f(Y_1^{[n]}), \ldots, f(Y_s^{[n]})]^T$, the TSRK methods (1.2) can be written in the following vector form

$$\begin{cases} Y^{[n]} = (u \otimes I_m) y_{n-2} + \big((e-u) \otimes I_m\big) y_{n-1} \\ \qquad + h\Big((A \otimes I_m) f(Y^{[n-1]}) + (B \otimes I_m) f(Y^{[n]}\Big), \\ y_n = \theta y_{n-2} + (1-\theta) y_{n-1} \\ \qquad + h\Big((v^T \otimes I_m) f(Y^{[n-1]}) + (w^T \otimes I_m) f(Y^{[n]})\Big), \end{cases} \tag{1.4}$$

where $e = [1, \ldots, 1]^T \in \mathbb{R}^s$ and I_m is the identity matrix of dimension m.

To analyze stability properties of (1.4) it is convenient to reformulate these formulas as general linear methods (GLMs) of the form

$$\left[\begin{array}{c} Y^{[n]} \\ \hline y_n \\ y_{n-1} \\ hf(Y^{[n]}) \end{array}\right] = \left[\begin{array}{c|ccc} B & e-u & u & A \\ \hline w^T & 1-\theta & \theta & v^T \\ 0 & 1 & 0 & 0 \\ I_s & 0 & 0 & 0 \end{array}\right] \left[\begin{array}{c} hf(Y^{[n]}) \\ \hline y_{n-1} \\ y_{n-2} \\ hf(Y^{[n-1]}) \end{array}\right]. \tag{1.5}$$

This representation corresponds to the problem (1.1) with $m = 1$ which is relevant in linear stability analysis. Putting

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|ccc} B & e-u & u & A \\ \hline w^T & 1-\theta & \theta & v^T \\ 0 & 1 & 0 & 0 \\ I_s & 0 & 0 & 0 \end{array}\right] \in \mathbb{R}^{(2s+2)\times(2s+2)}, \tag{1.6}$$

and applying (1.5) to the linear test equation

$$y' = \xi y, \quad t \geq 0, \tag{1.7}$$

where $\xi \in \mathbb{C}$, it follows that the stability properties of (1.5) with respect to (1.7) are determined by the stability matrix $\mathbf{M}(z)$ defined by

$$\mathbf{M}(z) = \mathbf{V} + z\mathbf{B}(\mathbf{I_s} - z\mathbf{A})^{-1}\mathbf{U}, \tag{1.8}$$

where $z = h\xi \in \mathbb{C}$. We also define the stability function $\tilde{p}(\omega, z)$ as the characteristic polynomial of $\mathbf{M}(z)$, i.e.,

$$\tilde{p}(\omega, z) = \det\Big(\omega I_{s+2} - \mathbf{M}(z)\Big). \tag{1.9}$$

This is a polynomial of degree $s+2$ with respect to ω whose coefficients are rational functions with respect to z. For methods for which the coefficient matrix B has a one point spectrum (1.3) it is more convenient to work with the function $p(\omega, z)$ defined by

$$p(\omega, z) = (1 - \lambda z)^s \tilde{p}(\omega, z), \tag{1.10}$$

in which the coefficients of ω^i, $i = 0, 1, \ldots, s+2$, are polynomials of degree s with respect to z.

In [1] the authors described the construction of TSRK methods for which the stability polynomial assumes the simple form

$$p(\omega, z) = \omega^s \Big((1 - \lambda z)^s \omega^2 - p_1(z)\omega + p_0(z) \Big), \tag{1.11}$$

with a root $\omega = 0$ of multiplicity s, where $p_1(z)$ and $p_0(z)$ are polynomials of degree s with respect to z. Methods for which this is the case are said to possess quadratic stability (QS). We were then aiming in [1] at construction of methods which are A-stable and L-stable. This leads to large systems of polynomial equations for the unknown coefficients of the methods which were then solved by least squares minimization. This approach works reasonably well if the number of stages s is not too large and in [1] examples of methods found in this way are given up to five stages. However, this is often not manageable when s is high. In fact, the authors were striving for high order methods with insufficient number of stages and as a result could not control the size of the error constant and the stability at infinity. On the contrary, the methods constructed in this paper do not suffer from these disadvantages: there are enough free parameters to obtain methods with small error constrants, reliable error estimates and good stability properties. In this paper we propose a completely different and a much simpler approach which is based on the so-called inherent quadratic stability (IQS). As will be explained later these are some conditions imposed on the coefficients matrices $\mathbf{A}$, $\mathbf{U}$, $\mathbf{B}$, and $\mathbf{V}$ which guarantee that the stability polynomial of the resulting method reduces to (1.11). These IQS conditions are easy to resolve, even for methods with quite large number of stages, without the need to solve complicated systems of nonlinear equations as was the case in [1]. This leads to methods with more accurate representation of coefficients than for methods constructed in [1]. It is also important to observe that quadratic stability is the most natural requirement for TSRK methods, as it will be afterward explained in the paper. The characterization of such methods, was inspired by the recent work on GLMs with inherent Runge-Kutta stability (IRKS) [14], [15], [16], [31], [32]. As in [1] we are aiming for methods which are A-stable and L-stable. This is accomplished with the aid of symbolic manipulation packages using the Schur criterion [28] (see also [27]) applied to the quadratic polynomial

$$(1-\lambda z)^s w^2 - p_1(z)\omega + p_0(z)$$

appearing in (1.11) for $\lambda > 0$. We are also investigating the possibility of constructing methods which are algebraically stable. This work will be reported in [19].

The organization of the paper is as follows. In Section 2 stage order and order conditions for TSRK methods are derived using the theory of GLMs for ODEs. In Section 3 the characterization of TSRK methods for which stability properties are determined by quadratic stability polynomials is obtained. This leads to the notion of inherent quadratic stability (IQS). The algorithm for the construction of such methods, with additional property that the coefficient matrix B has a one point spectrum, is then described in Section 4. In Section 6 the construction of A-stable and L-stable quadratic stability polynomials is discussed. The examples of TSRK methods with IQS and coefficient matrix B which has a one point spectrum are presented in Section 7. In Section 8 we present some numerical experiments for fixed stepsize implementations of classical Runge-Kutta-Gauss method of order $p=4$ and stage order $q=2$ and TSRK method of order $p=4$ and stage order $q=4$, and SDIRK method of order $p=3$ and stage order $q=2$ and TSRK method of order $p=3$ and stage order $q=3$. These results indicate that in contrast to Runge-Kutta formulas TSRK methods constructed in this paper do not suffer from order reduction for stiff problems. Finally, in Section 9 some concluding remarks are given and plans for future work are outlined.

2 Stage order and order conditions

In this section we derive the stage order and order conditions for TSRK methods (1.2) using the order theory for GLMs developed by Butcher [10]. Consider the GLM with s internal stages and r external stages of the form

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

$n=1,2,\ldots,N$, where $Y_i^{[n]}$ is an approximation to $y(t_{n-1}+c_i h)$ and $y_i^{[n]}$ is an approximation to the linear combination of the derivatives of the solution $y(t)$ to (1.1) at the point t_n. For TSRK methods (1.4) formulated as GLMs (1.5) we have $r=s+2$, $y_1^{[n]}=y_n$, $y_2^{[n]}=y_{n-1}$ and $y_i^{[n]}=hf(Y_{i-2}^{[n]})$,

$i = 3, 4, \ldots, s+2$. These methods are characterized by the abscissa vector $c = [c_1, \ldots, c_s]^T$ and four coefficient matrices $\mathbf{A} = [a_{ij}]$, $\mathbf{U} = [u_{ij}]$, $\mathbf{B} = [b_{ij}]$, and $\mathbf{V} = [v_{ij}]$, with

$$\mathbf{A} \in \mathbb{R}^{s\times s}, \quad \mathbf{U} \in \mathbb{R}^{s\times r}, \quad \mathbf{B} \in \mathbb{R}^{r\times s}, \quad \mathbf{V} \in \mathbb{R}^{r\times r}.$$

The representation of TSRK methods (1.2) as GLMs (2.1) was discussed in Section 1. This leads to the formula (1.5), where the vector $y^{[n]}$ of external approximations of GLM (2.1) is expressed in terms of the quantities y_n, y_{n-1} and $hf(Y^{[n]})$ of the TSRK method (1.2). This also leads to the representation (1.6), where the coefficient matrices $\mathbf{A}$, $\mathbf{U}$, $\mathbf{B}$, and $\mathbf{V}$ of GLM (2.1) are expressed in terms of the coefficients θ, u, v, w, A, and B of TSRK method (1.2).

To formulate the stage order and order conditions for GLM (2.1) we assume that the components of the input vector $y_i^{[n-1]}$ for the next step satisfy

$$y_i^{[n-1]} = \sum_{k=0}^{p} q_{ik} h^k y^{(k)}(t_{n-1}) + O(h^{p+1}), \quad i = 1, 2, \ldots, r, \tag{2.2}$$

for some real parameters q_{ik}, $i = 1, 2, \ldots, r$, $k = 0, 1, \ldots, p$. We then request that the components of the internal stages $Y_i^{[n]}$ are approximations of order $q \geq p-1$ to the solution $y(t)$ of (1.1) at the points $t_{n-1} + c_i h$, i.e.,

$$Y_i^{[n]} = y(t_{n-1} + c_i h) + O(h^{q+1}), \quad i = 1, 2, \ldots, r, \tag{2.3}$$

and that the components of the output vector $y_i^{[n]}$ satisfy

$$y_i^{[n]} = \sum_{k=0}^{p} q_{ik} h^k y^{(k)}(t_n) + O(h^{p+1}), \quad i = 1, 2, \ldots, r. \tag{2.4}$$

The integers q and p are called the stage order and order, respectively, of GLM (2.1). We collect the parameters q_{ik} appearing in (2.2) and (2.4) in the vectors $\mathbf{q}_k$ defined by

$$\mathbf{q}_k = \begin{bmatrix} q_{1k} & q_{2k} & \cdots & q_{rk} \end{bmatrix}^T \in \mathbb{R}^r, \quad k = 0, 1, \ldots, p.$$

We also introduce the notation $e^{cz} = \begin{bmatrix} e^{c_1 z} & e^{c_2 z} & \cdots & c^{c_s z} \end{bmatrix}^T$, and define the vector $\mathbf{w}(z)$ by

$$\mathbf{w}(z) = \sum_{k=0}^{p} \mathbf{q}_k z^k, \quad z \in \mathbb{C}.$$

Here, $\mathbb{C}$ is the set of complex numbers. We have the following theorem.

Theorem 2.1 *(Butcher [10]). Assume that $y^{[n-1]}$ satisfies (2.2). Then the GLM (2.1) of order p and stage order $q = p$ satisfies (2.3) and (2.4) if and only if*

$$e^{cz} = z\mathbf{A}e^{cz} + \mathbf{U}\mathbf{w}(z) + O(z^{p+1}), \tag{2.5}$$

and

$$e^{z}\mathbf{w} = z\mathbf{B}e^{cz} + \mathbf{V}\mathbf{w}(z) + O(z^{p+1}). \tag{2.6}$$

Expanding e^{cz} and e^z in (2.5) and (2.6) into power series around $z = 0$ and comparing the constant terms in the resulting expressions we obtain the preconsistency conditions

$$\mathbf{U}\mathbf{q}_0 = \mathbf{e}, \quad \mathbf{V}\mathbf{q}_0 = \mathbf{q}_0, \tag{2.7}$$

where $\mathbf{e} = [1, \dots, 1] \in \mathbb{R}^{s+2}$. Comparing the terms of order z^k, $k = 1, 2, \dots, p$ in the resulting expressions the stage order and order conditions can be reformulated in the form

$$\frac{c^k}{k!} - \frac{\mathbf{A}c^{k-1}}{(k-1)!} - \mathbf{U}\mathbf{q}_k = 0, \quad k = 1, 2, \dots, p, \tag{2.8}$$

and

$$\sum_{l=0}^{k} \frac{\mathbf{q}_{k-l}}{l!} - \frac{\mathbf{B}c^{k-1}}{(k-1)!} - \mathbf{V}\mathbf{q}_k = 0, \quad k = 1, 2, \dots, p, \tag{2.9}$$

compare also [23]. We determine next the vectors $\mathbf{q}_k$, $k = 0, 1, \dots, p$, appearing in (2.8) and (2.9). It follows from (1.5) that for TSRK method (1.2) the vector of external approximations $y^{[n]}$ assumes the form

$$y^{[n]} = \begin{bmatrix} y_n \\ y_{n-1} \\ hf(Y^{[n]}) \end{bmatrix} = \begin{bmatrix} y(t_n) \\ y(t_n - h) \\ y'(t_n + (c-e)h) \end{bmatrix} + O(h^{p+1}),$$

where $e = [1, \dots, 1] \in \mathbb{R}^s$, and expanding $y(t_n - h)$ and $y'(t_n + (c-e)h)$ into Taylor series around the point t_n we obtain

$$y^{[n]} = \begin{bmatrix} y(t_n) \\ y(t_n) - hy'(t_n) + \frac{h^2}{2!}y''(t_n) + \cdots + (-1)^p\frac{h^p}{p!}y^{(p)}(t_n) \\ hy'(t_n)e + h^2y''(t_n)\frac{(c-e)}{1!} + \cdots + h^py^{(p)}(t_n)\frac{(c-e)^{p-1}}{(p-1)!} \end{bmatrix} + O(h^{p+1}),$$

where $(c-e)^\nu$, $\nu = 0, 1, \dots, p-1$, is intended componentwise. Comparing this expression with (2.4) leads to the following formulas for the vectors $\mathbf{q}_k$

$$\mathbf{q}_0 = [1\ 1\ \mathbf{0}^T]^T, \quad \mathbf{q}_k = \begin{bmatrix} 0 & \frac{(-1)^k}{k!} & \left(\frac{(c-e)^{k-1}}{(k-1)!}\right)^T \end{bmatrix}^T,$$

$k = 1, 2, \ldots, p$, where $\mathbf{0}$ in $\mathbf{q}_0$ stands for the zero vector of dimension s. The vector $\mathbf{q}_0$ is called the preconsistency vector. It can be verified using the representation (1.6) that the preconsistency conditions (2.7) are automatically satisfied for TSRK method (1.2). The vector $\mathbf{q}_1$ is called the consistency vector and the conditions corresponding to $k = 1$ in (2.8) and (2.9) are called the consistency and stage consistency conditions. These conditions take the form

$$\mathbf{B}e + \mathbf{V}\mathbf{q}_1 = \mathbf{q}_0 + \mathbf{q}_1, \quad \mathbf{A}e + \mathbf{U}\mathbf{q}_1 = c.$$

It is convenient to express the stage order and order conditions (2.8) and (2.9) directly in terms of the coefficients c, θ, u, v, w, A, and B of the original TSRK methods (1.2). Theorem 2.1 implies the following result.

Theorem 2.2 *(compare [2], [24]) Assume that the TSRK method (1.2) or (1.4) has order p and stage order $q = p$. Then the order and stage order conditions take the form*

$$C_k := \frac{c^k}{k!} - \frac{(-1)^k}{k!}u - \frac{A(c-e)^{k-1}}{(k-1)!} - \frac{Bc^{k-1}}{(k-1)!} = 0, \qquad (2.10)$$

$k = 1, , 2, \ldots, p$, and

$$\hat{C}_k := \frac{1}{k!} - \frac{(-1)^k}{k!}\theta - \frac{v^T(c-e)^{k-1}}{(k-1)!} - \frac{w^T c^{k-1}}{(k-1)!} = 0, \qquad (2.11)$$

$k = 1, 2, \ldots, p$, where $c^\nu := [c_1^\nu, \ldots, c_s^\nu]^T$.

Putting $k = 1$ in (2.10) and (2.11) the stage consistency and consistency conditions take the form $(A + B)e - u = c$, $(v^T + w^T)e = 1 + \theta$.

3 Characterization of TSRK methods with quadratic stability

To investigate the form of the stability function of the method (1.2) it is convenient to introduce some equivalence relation between matrices of the same dimensions. We say that the two matrices D and E are equivalent, which will be denoted by $D \equiv E$, if they are equal except for the first two rows.

This relation has several useful properties which will aid in the derivation of TSRK methods with appropriate stability properties. It can be verified that if $F \in \mathbb{R}^{(\nu+2)\times(\nu+2)}$ is a matrix partitioned as follows

$$F = \left[\begin{array}{c|c} F_{11} & F_{12} \\ \hline F_{21} & F_{22} \end{array}\right],$$

where $F_{11} \in \mathbb{R}^{2\times 2}$, $F_{12} \in \mathbb{R}^{2\times\nu}$, $F_{21} \in \mathbb{R}^{\nu\times 2}$, $F_{22} \in \mathbb{R}^{\nu\times\nu}$, and if $F_{21} = 0$, then $D \equiv E$ implies $FD \equiv FE$. Moreover, for any matrix F we have also $D \equiv E$ implies $DF \equiv EF$.

In general, it is a very complicated task to construct TSRK methods (1.2) which possess QS, especially for methods with large number of stages s, since this requires the solution of large systems of polynomial equations of high degree, for the unknown coefficients of the methods. However, if we are willing to restrict the class of methods, it is possible to find interrelations between the coefficients matrices $\mathbf{A}$, $\mathbf{U}$, $\mathbf{B}$, and $\mathbf{V}$ defined by (1.6) which ensure that this is the case, i.e., that the TSRK method (1.2) possesses QS. Such conditions in the case of GLMs with Runge-Kutta stability were discovered recently by Butcher and Wright [15], [31], and lead to the concept of Inherent Runge–Kutta stability (IRKS). They take a similar form for TSRK methods with QS, leading to the concept of Inherent Quadratic Stability (IQS), formalized in the following definition.

Definition 3.1 *The TSRK method (1.2) with coefficients* $\mathbf{A}$*,* $\mathbf{U}$*,* $\mathbf{B}$*, and* $\mathbf{V}$ *defined by (1.6) has inherent quadratic stability (IQS) if there exists a matrix* $\mathbf{X} \in \mathbb{R}^{(s+2)\times(s+2)}$ *such that*

$$\mathbf{BA} \equiv \mathbf{XB}, \tag{3.1}$$

and

$$\mathbf{BU} \equiv \mathbf{XV} - \mathbf{VX}. \tag{3.2}$$

The significance of this definition follows from the following theorem.

Theorem 3.1 *Assume that the TSRK method (1.2) has IQS and that the matrices* $I_s - z\mathbf{A}$ *and* $I_{s+2} - z\mathbf{X}$ *are nonsingular. Then its stability function* $\tilde{p}(\omega, z)$ *defined by (1.9) assumes the form*

$$\tilde{p}(\omega, z) = \omega^s\Big(\omega^2 - \tilde{p}_1(z)\omega + \tilde{p}_0(z)\Big), \tag{3.3}$$

where $\tilde{p}_1(z)$ *and* $\tilde{p}_0(z)$ *are rational functions with respect to* z*.*

Proof: The proof of this theorem follows along the lines of the corresponding result for GLMs with IRKS [15], [31]. Assuming $\mathbf{I_s} - z\mathbf{A}$ nonsingular, the IQS relation (3.1) is equivalent to

$$\mathbf{B} \equiv (\mathbf{I}_{s+2} - z\mathbf{X})\mathbf{B}(\mathbf{I}_s - z\mathbf{A})^{-1}. \tag{3.4}$$

To investigate the characteristic polynomial of the corresponding matrix $\mathbf{M}(z)$, as defined in (1.8), it is more convenient to consider the matrix related to $\mathbf{M}(z)$ by similarity transformation. Using (3.2) and (3.4) and assuming that $\mathbf{I}_{s+2} - z\mathbf{X}$ is nonsingular, we obtain

$$(\mathbf{I}_{s+2} - z\mathbf{X})\mathbf{M}(z)(\mathbf{I}_{s+2} - z\mathbf{X})^{-1} \equiv \mathbf{V}. \tag{3.5}$$

It follows from the structure of the matrix $\mathbf{V}$ (see (1.6)) and the relation (3.5) that the matrix $(\mathbf{I}_{s+2} - z\mathbf{X})\mathbf{M}(z)(\mathbf{I}_{s+2} - z\mathbf{X})^{-1}$ can be partitioned as follows

$$(\mathbf{I}_{s+2} - z\mathbf{X})\mathbf{M}(z)(\mathbf{I}_{s+2} - z\mathbf{X})^{-1} = \left[\begin{array}{c|c} \tilde{M}_{11}(z) & \tilde{M}_{12}(z) \\ \hline 0 & 0 \end{array}\right], \tag{3.6}$$

where $\tilde{M}_{11}(z) \in \mathbb{R}^{2\times 2}$, $\tilde{M}_{12}(z) \in \mathbb{R}^{2\times s}$, and 0 stands for zero matrix of dimension $s \times 2$ and $s \times s$, respectively. This relation implies that the characteristic polynomial $\tilde{p}(\omega, z)$ of the matrix

$$(\mathbf{I}_{s+2} - z\mathbf{X})\mathbf{M}(z)(\mathbf{I}_{s+2} - z\mathbf{X})^{-1}$$

and $\mathbf{M}(z)$ assumes the form (3.3). $\square$

Observe that the matrices $I_s - z\mathbf{A}$ and $I_{s+2} - z\mathbf{X}$ are singular at a finite number of points in the complex plane. When we implement these methods, the stepsize control mechanism should check for those singular points and choose the stepsize so that $z = h\xi$ is far from them by some safe margin. This issue can be investigated using a similar approach to that used in [5] in the case of singly implicit Runge-Kutta methods.

The proof of Theorem 3.1 explains also the reason why it is natural in the context of TSRK methods to investigate quadratic stability. It follows that the stability matrix $\mathbf{M}(z)$ and the coefficient matrix $\mathbf{V}$ are related by the equation (3.5), where the matrix $\mathbf{M}(z)$ satisfies (3.6). Moreover, in the case of TSRK methods, the matrix $\mathbf{V}$ has a very precise structure given by the representation (1.6), and its eigenvalues are 1, $-\theta$ and 0 (with multiplicity s). Therefore, for $\theta \neq 0$, looking for a stability function of the type (1.11) is quite natural choice.

To express the IQS conditions (3.1) and (3.2) in terms of the coefficients θ, u, v, w, A, and B of TSRK method (1.2) we partition the matrix $\mathbf{X}$ as follows

$$\mathbf{X} = \left[\begin{array}{c|c} X_{11} & X_{12} \\ \hline X_{21} & X_{22} \end{array}\right], \tag{3.7}$$

where $X_{11} \in \mathbb{R}^{2\times 2}$, $X_{12} \in \mathbb{R}^{2\times s}$, $X_{21} \in \mathbb{R}^{s\times 2}$, $X_{22} \in \mathbb{R}^{s\times s}$. We also partition accordingly the matrices $\mathbf{B}$, $\mathbf{U}$, and $\mathbf{V}$ (see (1.6))

$$\mathbf{B} = \left[\begin{array}{c} B_{11} \\ \hline I_s \end{array}\right], \quad \mathbf{U} = \left[\begin{array}{c|c} U_{11} & A \end{array}\right], \quad \mathbf{V} = \left[\begin{array}{c|c} V_{11} & V_{12} \\ \hline 0 & 0 \end{array}\right],$$

where $B_{11} \in \mathbb{R}^{2\times s}$, $U_{11} \in \mathbb{R}^{s\times 2}$, $V_{11} \in \mathbb{R}^{2\times 2}$, $V_{12} \in \mathbb{R}^{2\times s}$ are given by

$$B_{11} = \begin{bmatrix} w^T \\ 0 \end{bmatrix}, U_{11} = \begin{bmatrix} e-u & u \end{bmatrix}, V_{11} = \begin{bmatrix} 1-\theta & \theta \\ 1 & 0 \end{bmatrix}, V_{12} = \begin{bmatrix} v^T \\ 0 \end{bmatrix},$$

and 0 in $\mathbf{V}$ stands for zero matrices of dimension $s\times 2$ and $s\times s$, respectively.

Theorem 3.2 *A TSRK method (1.2) has IQS if there exist vectors* $\alpha, \beta \in \mathbb{R}^s$ *and a matrix* $X \in \mathbb{R}^{s\times s}$ *such that the following conditions are statisfied*

$$B = \alpha w^T + X, \quad e = \alpha + \beta, \quad u = \theta\alpha, \quad A = \alpha v^T. \tag{3.8}$$

Proof: According to the way we have partitioned the above matrices, IQS conditions (3.1) and (3.2) are equivalent to

$$B = X_{21}B_{11} + X_{22},$$

and

$$U_{11} = X_{21}V_{11}, \quad A = X_{21}V_{12},$$

respectively. By setting

$$\begin{bmatrix} \alpha & \beta \end{bmatrix} = X_{21} \in \mathbb{R}^{s\times 2}, \quad X = X_{22}, \tag{3.9}$$

with $\alpha, \beta \in \mathbb{R}^s$, the theorem follows. □

The price we have to pay for IQS as compared with the approach presented in [1] is the increase by one in the number of stages for the same order and stage order. However, the approach based on IQS leads to a larger number of free parameters than that in [1], which can be utilized for other purposes such as, for example, the construction of reliable estimators of local discretization errors, and possibly the construction of TSRK methods which are also algebraically stable. These topics are the subject of current work [18], [19].

4 Construction of TSRK methods with IQS properties

We first compute the coefficient matrix A and the vector v from stage order and order conditions (2.10) and (2.11). Introducing the notation

$$C = \begin{bmatrix} c & \frac{c^2}{2!} & \cdots & \frac{c^s}{s!} \end{bmatrix}, \quad \tilde{C} = \begin{bmatrix} e & \frac{c}{1!} & \cdots & \frac{c^{s-1}}{(s-1)!} \end{bmatrix},$$

$$d = \begin{bmatrix} -1 & \frac{1}{2!} & \cdots & \frac{(-1)^s}{s!} \end{bmatrix}^T, \quad g = \begin{bmatrix} 1 & \frac{1}{2!} & \cdots & \frac{1}{s!} \end{bmatrix}^T,$$

$$E = \begin{bmatrix} e & \frac{c-e}{1!} & \cdots & \frac{(c-e)^{s-1}}{(s-1)!} \end{bmatrix},$$

the conditions (2.10) and (2.11) are equivalent to $AE = C - ud^T - B\tilde{C}$, and $v^T E = g^T - \theta d^T - w^T\tilde{C}$, respectively. We note that, by assuming distinct abscissas, the matrices C, $\tilde{C}$, and E are nonsingular because of Vandermonde type. Hence we obtain

$$A = (C - ud^T - B\tilde{C})E^{-1}, \tag{4.1}$$

and

$$v^T = (g^T - \theta d^T - w^T\tilde{C})E^{-1}. \tag{4.2}$$

To obtain TSRK methods with IQS we compute the matrix X from the first condition in (3.8), i.e., $X = B - \alpha w^T$, and the vectors β and u from the second and third condition of (3.8), i.e.,

$$\beta = e - \alpha, \quad u = \theta\alpha. \tag{4.3}$$

Then we enforce the last condition in (3.8) using the representations of A and v given by (4.1) and (4.2). This leads to

$$C - ud^T - B\tilde{C} = \alpha g^T - \theta\alpha d^T - \alpha w^T\tilde{C}$$

and, since $\tilde{C}$ is nonsingular, using the condition $u = \theta\alpha$ we obtain

$$B = (C - \alpha(g^T - w^T\tilde{C}))\tilde{C}^{-1}. \tag{4.4}$$

Computing the matrix B from (4.4) and then the matrix A from (4.1), where $u = \theta\alpha$, and the vector v from (4.2) we obtain a family of TSRK methods (1.2) of order $p = s$ and stage order $q = p$ which depends on the parameters θ, α, c and w. By construction these methods satisfy IQS conditions (3.8). We impose next the condition (1.3) that the matrix B has a one point spectrum $\sigma(B) = \{\lambda\}$, where λ will be chosen in such a way that the resulting method has some desirable stability properties. This is equivalent to the requirement that the characteristic polynomial of B assumes the simple form $\det(\omega I_s - B) = (\omega - \lambda)^s$. Since

$$\det(\omega I_s - B) = \sum_{k=0}^{s} b_k\omega^{s-k},$$

where $b_0 = 1$, $b_k = b_k(\theta, \alpha, c, w)$, $k = 1, 2, \ldots, s$, and

$$(\omega - \lambda)^s = \sum_{k=0}^{s} \binom{s}{k} (-1)^k\lambda^k\omega^{s-k}$$

this is equivalent to the system of equations

$$b_k(\theta, \alpha, c, w) = \binom{s}{k} (-1)^k\lambda^k, \quad k = 1, 2, \ldots, s. \tag{4.5}$$

Since it follows from (4.4) that

$$B = (C - \alpha g^T)\tilde{C}^{-1} + \alpha w^T,$$

the system (4.5) is linear with respect to w, and its solution leads, by virtue of Theorem 3.1, to methods for which stability polynomial $p(\omega, z)$ takes the form (1.11), i.e.,

$$p(\omega, z) = \omega^s \Big((1-\lambda z)^s \omega^2 - p_1(z)\omega + p_0(z) \Big). \tag{4.6}$$

The polynomials $p_1(z)$ and $p_0(z)$ appearing in $p(\omega, z)$ take the form

$$\begin{aligned} p_1(z) &= p_{10} + p_{11}z + \cdots + p_{1,s-1}z^{s-1} + p_{1s}z^s, \\ p_0(z) &= p_{00} + p_{01}z + \cdots + p_{0,s-1}z^{s-1} + p_{0s}z^s. \end{aligned} \tag{4.7}$$

Since, by (1.8)–(1.11),

$$p(\omega, 0) = \det(\omega I_{s+2} - \mathbf{V}) = \omega^s(\omega - 1)(\omega + \theta) = \omega^s(\omega^2 - p_1(0)\omega + p_0(0))$$

it follows that

$$p_1(0) = p_{10} = 1 - \theta, \quad p_0(0) = p_{00} = -\theta. \tag{4.8}$$

Therefore, the polynomials $p_1(z)$ and $p_2(z)$ now take the form

$$p_1(z) = 1 - \theta + p_{11}z + \cdots + p_{1,s}z^s,$$

$$p_0(z) = -\theta + p_{01}z + \cdots + p_{0,s}z^s.$$

For the method of order $p = s$ the stability polynomial $p(\omega, z)$ satisfies the condition

$$p(e^z, z) = O(z^{s+1}), \quad z \to 0. \tag{4.9}$$

Expanding (4.9) into power series around $z = 0$ it follows from (4.8) that the constant term vanishes, and comparing to zero terms of order z^k, $k = 1, 2, \ldots, s$, we obtain a system of s linear equations for the $2s$ coefficients p_{1j}, p_{0j}, $j = 1, 2 \ldots, s$, of the polynomials $p_1(z)$ and $p_0(z)$. This system has a family of solutions depending on λ, θ, and s additional parameters which may be chosen from p_{1j} and p_{0j}. Moreover we observe that, assuming A-stability, the L-stability requirement is equivalent to

$$\lim_{z\to\infty} \frac{p_1(z)}{(1-\lambda z)^s} = 0, \quad \lim_{z\to\infty} \frac{p_0(z)}{(1-\lambda z)^s} = 0,$$

which leads to the conditions

$$p_{1s} = 0, \quad p_{0s} = 0. \tag{4.10}$$

The last point is now the computation of the vector α, which can be carried out comparing the expression of the stability polynomial now computed with the one coming from (3.6), i.e.

$$\tilde{p}(\omega, z) = \omega^s \det(\omega I_2 - \tilde{M}_{11}(z)). \tag{4.11}$$

Since the IQS conditions (3.8) do not depend on the blocks X_{11} and X_{12} of the matrix $\mathbf{X}$ in (3.7) we can assume without loss of generality that $X_{11} = 0$ and $X_{12} = 0$. Therefore, it follows from (3.6) that

$$\left[\begin{array}{c|c} I_2 & 0 \\ \hline -zX_{21} & I_2 - zX_{22} \end{array}\right] \left[\begin{array}{c|c} M_{11}(z) & M_{12}(z) \\ \hline M_{21}(z) & M_{22}(z) \end{array}\right]$$
$$= \left[\begin{array}{c|c} \tilde{M}_{11}(z) & \tilde{M}_{12}(z) \\ \hline 0 & 0 \end{array}\right] \left[\begin{array}{c|c} I_2 & 0 \\ \hline -zX_{21} & I_2 - zX_{22} \end{array}\right].$$

Hence,

$$M_{11}(z) = \tilde{M}_{11}(z) - z\tilde{M}_{12}(z)X_{21}, \quad M_{12}(z) = \tilde{M}_{12}(z)(I_2 - zX_{22}),$$

which, taking into account (3.9), leads to the following formula for the matrix $\tilde{M}_{11}(z)$

$$\tilde{M}_{11}(z) = M_{11}(z) + zM_{12}(z)(I_2 - zX)^{-1}[\ \alpha \quad \beta\ ], \tag{4.12}$$

where we recall $X = X_{22}$.

The construction of highly stable TSRK methods (1.2) with IQS properties and coefficient matrix B with one point spectrum $\sigma(B) = \{\lambda\}$ can be summarized in the following algorithm.

1. Choose the abscissa vector c with distinct components, such that the matrices $\tilde{C}$ and E defined at the beginning of this section are nonsingular.

2. We solve the system arising from (4.9) by fixing s coefficients of the polynomials $p_0(z)$ and $p_1(z)$ and deriving the remaining s as functions of θ and λ. Choose the parameters θ and $\lambda > 0$ so that the stability polynomial $p(\omega, z)$ is A-stable and also L-stable, by using the Schur criterion. This will be performed in Section 6 for s up to 8.

3. Compute the coefficient matrix B from the formula (4.4). This matrix depends on the vectors α and w.

4. Compute the vectors β and u from the second and third condition of (3.8), i.e., $\beta = e - \alpha$ and $u = \theta\alpha$.

5. Compute the coefficient matrix A from (4.1) and the vector v from (4.2). They depend on α and w.

6. Solve the system (4.5) with respect to w. This leads to a family of methods with IQS for which the matrix B has a one point spectrum $\sigma(B) = \{\lambda\}$.

7. Compute the matrix $\tilde{M}_{11}(z)$ from the relation (4.12), the stability polynomial $\tilde{p}(\omega, z)$ from (4.12) and $p(\omega, z) = (1 - \lambda z)^s \tilde{p}(\omega, z)$, whose coefficients p_{1j} and p_{0j} depend only on α.

8. Having computed the coefficients of the method in points 3, 4 and 5 such that the order conditions are satisfied up to order and stage order $p = q = s$, (4.9) is automatically satisfied by the polynomial $p(\omega, z)$ obtained in point 7. Then, in order to equate such stability polynomial with the one derived in point 2, it is sufficient to determine the parameter vector α by equalizing the s coefficients which have been fixed in point 2.

5 Construction of high order TSRK methods with IQS property

Unfortunately, the construction of higher order methods ($p = s \geq 7$) by using the algorithm presented in the previous section, and in particular the generation of the system of nonlinear equations in the parameter vector α, exceeds the capabilities of symbolic manipulation packages and in this section we describe an alternative approach to generate such nonlinear system, using some variants of the Fourier series method, proposed by Butcher and Jackiewicz [12] in the context of diagonally implicit multistage integration methods (DIMSIMs). The systems obtained in this way will then be solved by algorithms based on least squares minimization. Using this algorithm we were able to obtain A-stable and L-stable TSRK methods (1.2) of order and stage order $p = q = s = 7$ and $p = q = s = 8$, and such that the matrix B has a one point spectrum $\sigma(B) = \{\lambda\}$.

We denote by

$$q(\omega, z) = (1 - \lambda z)^s \omega^2 - p_1(z)\omega + p_0(z),$$

the quadratic factor in the stability polynomial (4.6). A Fourier series approach described in [12] can be summarized as follows. Assume that ω_μ, $\mu = 1, \ldots, N_1$, are complex numbers uniformely distributed on the unit circle. Multiplying the relation

$$q(\omega_\mu, z) = (1 - \lambda z)^s \omega_\mu^2 - p_1(z)\omega_\mu + p_0(z),$$

by ω_μ^{-k}, $k = 0, 1$, and summing with respect to μ, we obtain the following representations of the coefficients $p_0(z)$ and $p_1(z)$:

$$p_0(z) = \frac{1}{N_1} \sum_{\mu=1}^{N_1} q(\omega_\mu, z),$$
$$p_1(z) = -\frac{1}{N_1} \sum_{\mu=1}^{N_1} q(\omega_\mu, z).$$

Assume next that z_ν, $\nu = 1, \ldots, N_2$, are complex numbers uniformely distributed on the unit circle. Since the functions $p_0(z)$ and $p_1(z)$ have the form (4.7), we multiply

$$p_k(z_\nu) = p_{k0} + p_{k1} z_\nu + \cdots + p_{ks} z_\nu^s$$

by z_ν^{-l}, $l = 0, 1, \ldots, s$, and sum with respect to ν, obtaining

$$\begin{aligned} p_{0l} &= \frac{1}{N_1 N_2} \sum_{\mu=1}^{N_1} \sum_{\nu=1}^{N_2} z_\nu^{-l} q(\omega_\mu, z_\nu), \\ p_{1l} &= -\frac{1}{N_1 N_2} \sum_{\mu=1}^{N_1} \sum_{\nu=1}^{N_2} \omega_\mu^{-1} z_\nu^{-l} q(\omega_\mu, z_\nu). \end{aligned} \tag{5.1}$$

The nonlinear system determined in point 8 of Section 4 can be equivalently solved by using the expressions (5.1) of the coefficients p_{0l} and p_{1l}, if the integers N_1 and N_2 are chosen to be sufficiently large.

6 Construction of highly stable quadratic stability polynomials

In this section, in agreement with point 2 of the algorithm reported in the previous section, we derive methods of order $p = q = s$ with quadratic stability polynomials which are A-stable and L-stable for s up to 8. According to point 2 of the algorithm we will need to fix s coefficients of the polynomials $p_0(z)$ and $p_1(z)$: we choose to annihilate

$$p_{0l}, \quad l = l_0, \ldots, s, \quad p_{1l}, \quad l = l_1, \ldots, s, \tag{6.1}$$

with $l_0 = \lceil \frac{s+1}{2} \rceil$ and $l_1 = \lfloor \frac{s+1}{2} \rfloor + 1$.

For $s = 1$ the stability polynomial (1.11) takes the form

$$p(\omega, z) = \omega\Big((1 - \lambda z)\omega^2 - p_1(z)\omega + p_0(z)\Big),$$

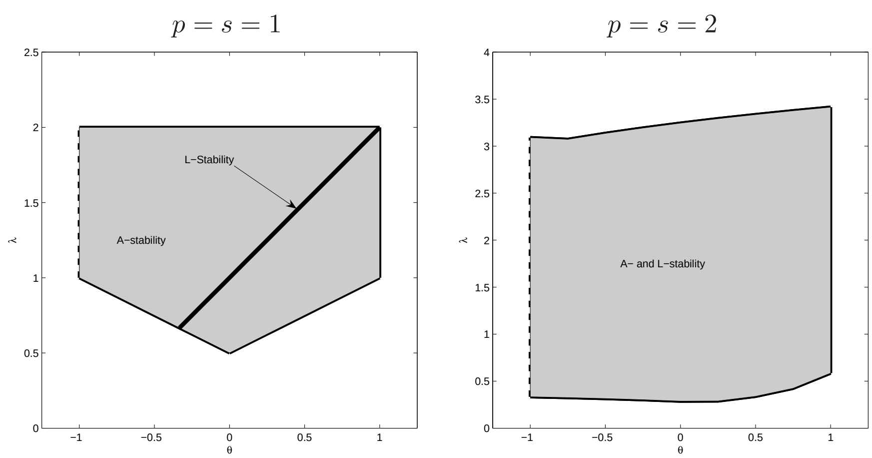

Figure 1: Regions of A-stability and L-stability in the (θ, λ)-plane for $p(\omega, z)$ with $p = s = 1$ and $p = s = 2$.

with $p_1(z) = 1 - \theta + p_{11}z$, $p_0(z) = -\theta + p_{01}z$. The solution of the equation corresponding to (4.9) with $s = 1$ is $p_{11} = 1 - \lambda - p_{01} + \theta$. Assuming, according to (6.1), that $p_{01} = 0$ it can be verified using the Schur criterion [28], [27] that $p(\omega, z)$ is A-stable if and only if $2\lambda + \theta \geq 1$, $2\lambda - \theta \geq 1$ and $\lambda \leq 2$. Moreover, $p_{11} = 0$ leads to $\theta = \lambda - 1$ and the resulting polynomial is L-stable if and only if $\frac{2}{3} \leq \lambda \leq 2$. This is illustrated in Fig. 1, where the range of parameters (θ, λ) for which $p(\omega, z)$ is A-stable corresponds to the shaded region and the range of (θ, λ) for which $p(\omega, z)$ is L-stable is plotted by a thick line.

For $s = 2, 3, \ldots, 8$, we are looking for A-stable methods which are also L-stable. This is the case if the degrees of the polynomials $p_0(z)$ and $p_1(z)$ in (1.11) are equal to $s - 1$, according to (4.10). For $s = 2$ the stability polynomial (1.11) takes the form

$$p(\omega, z) = \omega^2\Big((1 - \lambda z)^2\omega^2 - p_1(z)\omega + p_0(z)\Big),$$

with $p_1(z) = 1 - \theta + p_{11}z$ and $p_0(z) = -\theta + p_{01}z$. The system of equations corresponding to (4.9) with $s = 2$ takes the form

$$p_{11} - p_{01} = 1 - 2\lambda + \theta, \quad 2p_{11} = 3 - 8\lambda + 2\lambda^2 + \theta.$$

and the unique solution to this system is given by

$$p_{11} = \frac{3 - 8\lambda + 2\lambda^2 + \theta}{2}, \quad p_{01} = \frac{1 - 4\lambda + 2\lambda^2 - \theta}{2}.$$

The range of parameters (θ, λ) for which the $p(\omega, z)$ is A-stable and also L-stable is plotted in Fig. 1 by the shaded region.

For $s = 3$ the stability polynomial (1.11) takes the form

$$p(\omega, z) = \omega^3\Big((1-\lambda z)^3\omega^2 - p_1(z)\omega + p_0(z)\Big),$$

with $p_1(z) = 1 - \theta + p_{11}z + p_{12}z^2$ and $p_0(z) = -\theta + p_{01}z + p_{02}z^2$. The system of equations corresponding to (4.9) with $s = 3$ takes the form

$$p_{11} - p_{01} = 1 - 3\lambda + \theta, \quad 2p_{11} - 2p_{02} + 2p_{12} = 3 - 12\lambda + 6\lambda^2 + \theta,$$
$$3p_{11} + 6p_{12} = 7 - 36\lambda + 36\lambda^2 - 6\lambda^3 + \theta,$$

and assuming, according to (6.1), that $p_{02} = 0$, the unique solution to this system is given by

$$p_{11} = \frac{2(1 - 9\lambda^2 + 3\lambda^3 + \theta)}{3}, \quad p_{12} = \frac{5 - 36\lambda + 54\lambda^2 - 12\lambda^3 - \theta}{6},$$
$$p_{01} = \frac{1 - 9\lambda + 18\lambda^2 - 6\lambda^3 + \theta}{3}.$$

The range of parameters (θ, λ) for which the $p(\omega, z)$ is A-stable and also L-stable is plotted in Fig. 2 by the shaded region.

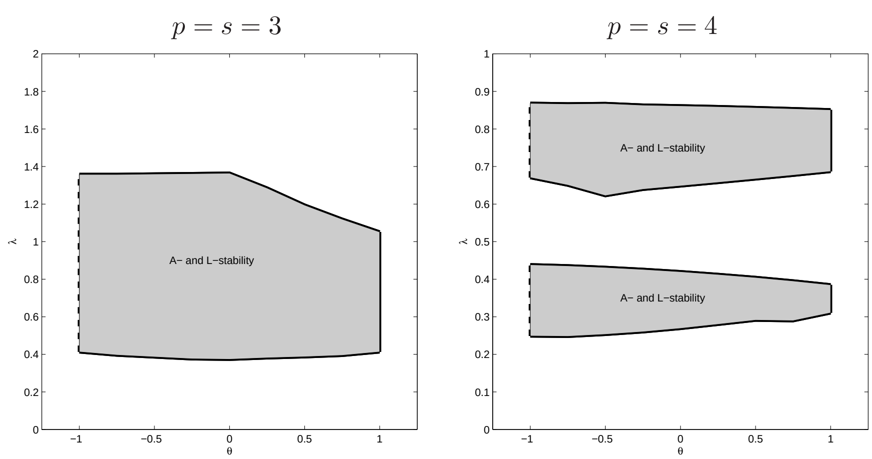

Figure 2: Regions of A-stability and L-stability in the (θ, λ)-plane for $p(\omega, z)$ with $p = s = 3$ and $p = s = 4$.

For $s = 4$ the stability polynomial (1.11) takes the form

$$p(\omega, z) = \omega^4\Big((1-\lambda z)^4\omega^2 - p_1(z)\omega + p_0(z)\Big),$$

with $p_1(z) = 1-\theta+p_{11}z+p_{12}z^2+p_{13}z^3$ and $p_0(z) = -\theta+p_{01}z+p_{02}z^2+p_{03}z^3$. The system of equations corresponding to (4.9) with $s = 4$ takes the form

$$p_{11} - p_{01} = 1 - 4\lambda + \theta, \quad 2p_{11} + 2p_{12} - 2p_{02} = 3 - 16\lambda + 12\lambda^2 + \theta,$$

$$3p_{11} + 6p_{12} + 6p_{13} - 6p_{03} = 7 - 48\lambda + 72\lambda^2 - 24\lambda^3 + \theta,$$

$$4p_{11} + 12p_{12} + 24p_{13} = 15 - 128\lambda + 288\lambda^2 - 192\lambda^3 + 24\lambda^4 + \theta,$$

and assuming, according to (6.1), that $p_{13} = 0$ and $p_{03} = 0$ the unique solution to this system is given by

$$p_{11} = \frac{1 - 32\lambda + 144\lambda^2 - 144\lambda^3 + 24\lambda^4 - \theta}{2},$$

$$p_{12} = \frac{17 - 192\lambda + 576\lambda^2 - 480\lambda^3 + 72\lambda^4 - \theta}{12},$$

$$p_{01} = \frac{3 - 40\lambda + 144\lambda^2 - 144\lambda^3 + 24\lambda^4 + \theta}{2},$$

$$p_{02} = \frac{7 - 96\lambda + 360\lambda^2 - 384\lambda^3 + 72\lambda^4 + \theta}{12}.$$

The range of parameters (θ, λ) for which the $p(\omega, z)$ is A-stable and also L-stable is plotted in Fig. 2 by the shaded region. The regions for $s = 2$, 3, and 4 were obtained by computer searches in the parameter space (θ, λ) using the Schur criterion [28], [27].

For $s = 5$ the stability polynomial (1.11) takes the form

$$p(\omega, z) = \omega^5\Big((1 - \lambda z)^5\omega^2 - p_1(z)\omega + p_0(z)\Big),$$

with $p_1(z) = 1 - \theta + p_{11}z + p_{12}z^2 + p_{13}z^3 + p_{14}z^4$ and $p_0(z) = -\theta + p_{01}z + p_{02}z^2 + p_{03}z^3 + p_{04}z^4$. The system of equations corresponding to (4.9) with $s = 5$ takes the form

$$p_{11} - p_{01} = 1 - 5\lambda + \theta, \quad p_{11} + p_{12} - p_{02} = 3/2 - 10\lambda + 10\lambda^2 + \theta/2,$$

$$3p_{11} + 6p_{12} + 6p_{13} - 6p_{03} = 7 - 60\lambda + 120\lambda^2 - 60\lambda^3 + \theta,$$

$$4p_{11} + 12p_{12} + 24p_{13} + 24p_{14} - 24p_{04} = 15 - 160\lambda + 480\lambda^2 - 480\lambda^3 + 120\lambda^4 + \theta$$

$$5p_{11} + 20p_{12} + 60p_{13} + 120p_{14} = 31 - 400\lambda + 1600\lambda^2 - 2400\lambda^3 + 1200\lambda^4 - 120\lambda^5 + \theta$$

and assuming, according to (6.1), that $p_{03} = 0$, $p_{04} = 0$ and $p_{14} = 0$, the unique solution to this system is given by

$$p_{11} = \frac{13 - 200\lambda + 1200\lambda^2 - 3000\lambda^3 + 2400\lambda^4 - 360\lambda^5 + 3\theta}{5},$$

$$p_{12} = \frac{-13 + 400\lambda - 3200\lambda^2 + 8400\lambda^3 - 6600\lambda^4 + 960\lambda^5 - 3\theta}{20},$$
$$p_{13} = \frac{31 - 600\lambda + 3600\lambda^2 - 7800\lambda^3 + 5400\lambda^4 - 720\lambda^5 + \theta}{60},$$
$$p_{01} = \frac{8 - 175\lambda + 1200\lambda^2 - 3000\lambda^3 + 2400\lambda^4 - 360\lambda^5 - 2\theta}{5},$$
$$p_{02} = \frac{9 - 200\lambda + 1400\lambda^2 - 3600\lambda^3 + 3000\lambda^4 - 480\lambda^5 - \theta}{20}.$$

the range of parameters (θ, λ) for which the polynomial $p(\omega, z)$ is A-stable and also L-stable is plotted in Fig. 3 by the shaded region.

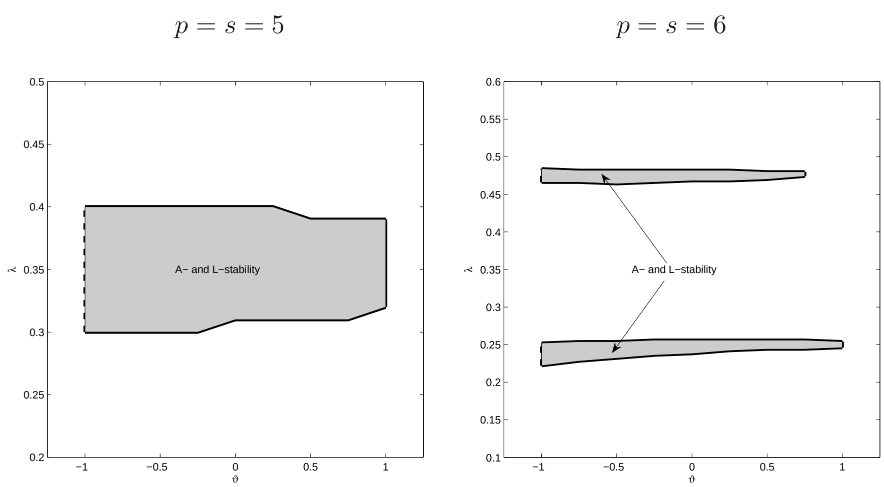

Figure 3: Regions of A-stability and L-stability in the (θ, λ)-plane for $p(\omega, z)$ with $p = s = 5$ and $p = s = 6$.

For $s = 6$ the stability polynomial (1.11) takes the form

$$p(\omega, z) = \omega^6 \Big((1 - \lambda z)^6 \omega^2 - p_1(z)\omega + p_0(z) \Big),$$

with $p_1(z) = 1 - \theta + p_{11}z + p_{12}z^2 + p_{13}z^3 + p_{14}z^4 + p_{15}z^5$ and $p_0(z) = -\theta + p_{01}z + p_{02}z^2 + p_{03}z^3 + p_{04}z^4 + p_{05}z^5$. Assuming, according to (6.1), that $p_{05} = 0$, $p_{04} = 0$, $p_{15} = 0$ and $p_{14} = 0$, the system of equations corresponding to (4.9) with $s = 6$ takes the form

$$p_{11} - p_{01} = 1 - 6\lambda + \theta, \quad p_{11} + p_{12} - p_{02} = 3/2 - 12\lambda + 15\lambda^2 + \theta/2,$$

$$3p_{11}+6p_{12}+6p_{13}-6p_{03}=7-72\lambda+180\lambda^2-120\lambda^3+\theta,$$
$$4p_{11}+12p_{12}+24p_{13}=15-192\lambda+720\lambda^2-960\lambda^3+360\lambda^4+\theta,$$
$$5p_{11}+20p_{12}+60p_{13}=31-480\lambda+2400\lambda^2-4800\lambda^3+3600\lambda^4-720\lambda^5+\theta,$$

$$\begin{aligned}6p_{11}+30p_{12}+120p_{13} &= 63-1152\lambda+7200\lambda^2-19200\lambda^3+21600\lambda^4\\ &- 8640\lambda^5+720\lambda^6+\theta.\end{aligned}$$

The range of parameters (θ,λ) for which the polynomial $p(\omega,z)$ is A-stable and also L-stable is plotted in Fig. 3 by the shaded region.

For $s=7$ the stability polynomial (1.11) takes the form

$$p(\omega,z)=\omega^7\Big((1-\lambda z)^7\omega^2-p_1(z)\omega+p_0(z)\Big),$$

with $p_1(z)=1-\theta+p_{11}z+p_{12}z^2+p_{13}z^3+p_{14}z^4+p_{15}z^5+p_{16}z^6$ and $p_0(z)=-\theta+p_{01}z+p_{02}z^2+p_{03}z^3+p_{04}z^4+p_{05}z^5+p_{06}z^6$. Assuming, according to (6.1), that $p_{06}=0$, $p_{05}=0$, $p_{04}=0$, $p_{16}=0$ and $p_{15}=0$, the system of equations corresponding to (4.9) with $s=7$ takes the form

$$\begin{aligned}
&p_{11}-p_{01}=1-7\lambda+\theta,\\
&p_{11}+p_{12}-p_{02}=3/2-14\lambda+21\lambda^2+\theta/2,\\
&3p_{11}+6p_{12}+6p_{13}-6p_{03}=7-84\lambda+252\lambda^2-210\lambda^3+\theta,\\
&4p_{11}+12p_{12}+24p_{13}+24p_{14}\\
&\qquad= 15-224\lambda+1008\lambda^2-1680\lambda^3+840\lambda^4+\theta,\\
&5p_{11}+20p_{12}+60p_{13}+120p_{14}\\
&\qquad= 31-560\lambda+3360\lambda^2-8400\lambda^3+8400\lambda^4-2520\lambda^5+\theta,\\
&6p_{11}+30p_{12}+120p_{13}+360p_{14}\\
&\qquad= 63-1344\lambda+10080\lambda^2-33600\lambda^3+50400\lambda^4\\
&\qquad\quad -30240\lambda^5+5040\lambda^6+\theta,\\
&7p_{11}+42p_{12}+210p_{13}+840p_{14}\\
&\qquad= 127-3136\lambda+28224\lambda^2-117600\lambda^3+235200\lambda^4\\
&\qquad\quad -211680\lambda^5+70560\lambda^6-5040\lambda^7+\theta.
\end{aligned}$$

The range of parameters (θ,λ) for which the $p(\omega,z)$ is A-stable and also L-stable is plotted in Fig. 4 by the shaded region.

For $s=8$ the stability polynomial (1.11) takes the form

$$p(\omega,z)=\omega^8\Big((1-\lambda z)^8\omega^2-p_1(z)\omega+p_0(z)\Big),$$

with $p_1(z)=1-\theta+p_{11}z+p_{12}z^2+p_{13}z^3+p_{14}z^4+p_{15}z^5+p_{16}z^6+p_{17}z^7$ and $p_0(z)=-\theta+p_{01}z+p_{02}z^2+p_{03}z^3+p_{04}z^4+p_{05}z^5+p_{06}z^6+p_{07}z^7$. Assuming, according to (6.1), that $p_{07}=0$, $p_{06}=0$, $p_{05}=0$, $p_{17}=0$,

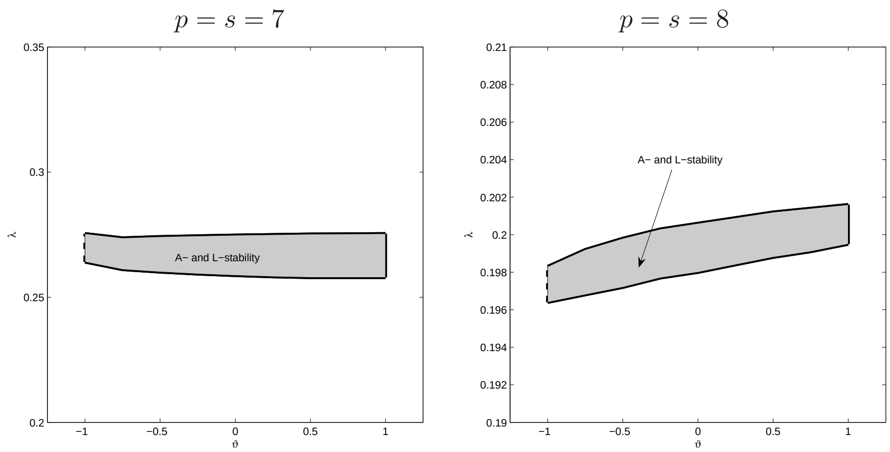

Figure 4: Regions of A-stability and L-stability in the (θ, λ)-plane for $p(\omega, z)$ with $p = s = 7$ and $p = s = 8$.

$p_{16} = 0$ and $p_{15} = 0$, the system of equations corresponding to (4.9) with $s = 8$ takes the form

$$
\begin{aligned}
& p_{11} - p_{01} = 1 - 8\lambda + \theta, \\
& p_{11} + p_{12} - p_{02} = 3/2 - 16\lambda + 28\lambda^2 + \theta/2, \\
& 3p_{11} + 6p_{12} + 6p_{13} - 6p_{03} = 7 - 96\lambda + 336\lambda^2 - 336\lambda^3 + \theta, \\
& 4p_{11} + 12p_{12} + 24p_{13} + 24p_{14} - 24p_{04} \\
& \quad = \ 15 - 256\lambda + 1344\lambda^2 - 2688\lambda^3 + 1680\lambda^4 + \theta, \\
& 5p_{11} + 20p_{12} + 60p_{13} + 120p_{14} \\
& \quad = \ 31 - 640\lambda + 4480\lambda^2 - 13440\lambda^3 + 16800\lambda^4 - 6720\lambda^5 + \theta, \\
& 6p_{11} + 30p_{12} + 120p_{13} + 360p_{14} \\
& \quad = \ 63 - 1536\lambda + 13440\lambda^2 - 53760\lambda^3 + 100800\lambda^4 \\
& \qquad - 80640\lambda^5 + 20160\lambda^6 + \theta, \\
& 7p_{11} + 42p_{12} + 210p_{13} + 840p_{14} \\
& \quad = \ 127 - 3584\lambda + 37632\lambda^2 - 188160\lambda^3 + 470400\lambda^4 \\
& \qquad - 564480\lambda^5 + 282240\lambda^6 - 40320\lambda^7 + \theta, \\
& 8p_{11} + 56p_{12} + 336p_{13} + 1680p_{14} \\
& \quad = \ 255 - 8192\lambda + 100352\lambda^2 - 602112\lambda^3 + 1881600\lambda^4 \\
& \qquad - 3010560\lambda^5 + 2257920\lambda^6 - 645120\lambda^7 + 40320\lambda^8 + \theta.
\end{aligned}
$$

The range of parameters (θ, λ) for which the polynomial $p(\omega, z)$ is A-stable and also L-stable is plotted in Fig. 4 by the shaded region.

All the systems listed above admit a unique solution. These solutions

$p=s$	A-stability and L-stability
1	$\lambda=1$
2	$\lambda\in[0.29,3.24]$
3	$\lambda\in[0.38,1.36]$
4	$\lambda\in[0.27,0.42]\cup[0.65,0.86]$
5	$\lambda\in[0.31,0.40]$
6	$\lambda\in[0.24,0.25]\cup[0.47,0.48]$
7	$\lambda\in[0.26,0.27]$
8	$\lambda\in[0.198,0.2]$

Table 6.1: Intervals of A-stability and L-stability corresponding to $\theta=0$ with restriction (6.1) on p_{kl}, with the additional condition $p_{11}=0$ in the case $s=1$.

for $s=6,7,8$ are not listed here and can be obtained from the authors.

7 Examples of TSRK methods with IQS

In this section we will follow the algorithm described in Section 4 to derive examples of A-stable and L-stable TSRK methods (1.2) with IQS and for which the coefficient matrix B has a one point spectrum $\sigma(B)=\{\lambda\}$. These examples correspond to $p=q=s$, up to $s=8$. It is always assumed that $\theta=0$ which implies that $u=0$, see (4.3).

Example 1. TSRK methods with $p=q=s=1$. The coefficients of the method corresponding to $\lambda=1$ and arbitrary abscissa c are given by

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

The stability polynomial $p(\omega,z)$ of this family of methods is

$$p(\omega,z)=\omega\big((1-z)\omega-1\big)$$

for any c. In particular, for $c=1$ this method is equivalent to the backward Euler method.

Example 2. TSRK methods with $p=q=s=2$. The coefficients of the method corresponding to $\lambda=\frac{5}{4}$ and abscissa vector $c=[0,1]^T$ are given by

$$\begin{array}{c|c|c} u & A & B \\ \hline \theta & v^T & w^T \end{array} = \begin{array}{c|cc|cc} 0 & -\frac{25}{32} & -\frac{25}{32} & \frac{75}{32} & -\frac{25}{32} \\ 0 & -\frac{11}{32} & -\frac{11}{32} & \frac{49}{32} & \frac{5}{32} \\ \hline 0 & -\frac{11}{32} & -\frac{11}{32} & \frac{49}{32} & \frac{5}{32} \end{array}.$$

The stability polynomial $p(\omega, z)$ of this method is

$$p(\omega, z) = \omega^2 \Big(\Big(1 - \frac{5}{4}z\Big)^2 \omega^2 - \Big(1 - \frac{31}{16}z\Big)\omega - \frac{7}{16}z \Big).$$

Example 3. TSRK methods with $p = q = s = 3$. The coefficients of the method corresponding to $\lambda = \frac{3}{4}$ and abscissa the vector $c = [0, \frac{1}{2}, 1]^T$ are given by $u = 0$, $\theta = 0$,

$$A = \begin{bmatrix} \frac{1371718}{2008359} & -\frac{1349029}{610487} & -\frac{598537}{334774} \\ \frac{1996151}{1120476} & -\frac{3899713}{676582} & -\frac{4599017}{986185} \\ \frac{2289675}{1145977} & -\frac{2640065}{408409} & -\frac{4106281}{785118} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{3955778}{915873} & -\frac{573724}{492365} & \frac{253229}{1575340} \\ \frac{4717083}{411104} & -\frac{3938351}{1455396} & \frac{307583}{814540} \\ \frac{6683188}{522061} & -\frac{3272705}{1193527} & \frac{472108}{741259} \end{bmatrix},$$

$$v = \begin{bmatrix} \frac{2289675}{1145977} & -\frac{2640065}{408409} & -\frac{4106281}{785118} \end{bmatrix}^T,$$

$$w = \begin{bmatrix} \frac{6683188}{522061} & -\frac{3272705}{1193527} & \frac{472108}{741259} \end{bmatrix}^T.$$

The stability polynomial $p(\omega, z)$ of this method is

$$p(\omega, z) = \omega^3 \Big(\Big(1 - \frac{3}{4}z\Big)^3 \omega^2 - \Big(1 - \frac{179}{96}z + \frac{53}{96}z^2\Big)\omega - \frac{59}{96}z \Big).$$

Example 4. TSRK methods with $p = q = s = 4$. The coefficients of the method corresponding to $\lambda = \frac{1}{3}$ and the abscissa vector $c = [0, \frac{1}{3}, \frac{2}{3}, 1]^T$ are given by

$$A = \begin{bmatrix} -\frac{73571}{418565} & \frac{316790}{450193} & -\frac{383309}{370547} & -\frac{1102057}{1459404} \\ -\frac{324116}{495273} & \frac{3108022}{1186313} & -\frac{2008351}{521461} & -\frac{1905671}{677809} \\ -\frac{813738}{787901} & \frac{4021146}{972541} & -\frac{6409321}{1054477} & -\frac{6349415}{1430988} \\ -\frac{426460}{370257} & \frac{4154204}{900915} & -\frac{12185608}{1797671} & -\frac{6621076}{1338039} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{1082275}{789096} & -\frac{47158}{1102905} & -\frac{20658}{230377} & \frac{16548}{733283} \\ \frac{2053468}{392523} & \frac{173881}{1660851} & -\frac{337517}{836884} & \frac{86197}{880374} \\ \frac{13765224}{1684843} & \frac{119918}{620675} & -\frac{387828}{932779} & \frac{214966}{1621163} \\ \frac{8694859}{954168} & \frac{68987}{727614} & -\frac{198815}{935168} & \frac{90358}{331129} \end{bmatrix},$$

$$v = \left[\begin{array}{cccc} -\frac{426460}{370257} & \frac{4154204}{900915} & -\frac{12185608}{1797671} & -\frac{6621076}{1338039} \end{array} \right]^T,$$

$$w = \left[\begin{array}{cccc} \frac{8694859}{954168} & \frac{68987}{727614} & -\frac{198815}{935168} & \frac{90358}{331129} \end{array} \right]^T.$$

The stability polynomial $p(\omega, z)$ of this method is

$$p(\omega, z) = \omega^4 \Big(\Big(1 - \frac{1}{3}z\Big)^4 \omega^2 - p_1(z)\omega + p_0(z) \Big)$$

with

$$p_1(z) = 1 - \frac{744347}{1148421}z + \frac{2965}{320219}z^2, \quad p_0(z) = -\frac{241021}{765596}z - \frac{198226}{1427227}z^2.$$

Example 5. TSRK methods with $p = q = s = 5$. The coefficients of the method corresponding to $\lambda = \frac{7}{20}$ and the abscissa vector $c = [0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1]^T$ are given by

$$A = \left[\begin{array}{ccccc} \frac{-910895}{2636314} & \frac{1530449}{1462933} & \frac{80731}{858808} & \frac{-6732586}{1712163} & \frac{-1286173}{3283870} \\ \frac{-2876560}{3965691} & \frac{1052194}{479091} & \frac{351641}{1781853} & \frac{-16016705}{1940229} & \frac{-553297}{672917} \\ \frac{-973540}{873967} & \frac{3166258}{938781} & \frac{137149}{452544} & \frac{-17304128}{1364977} & \frac{-373097}{295475} \\ \frac{-2881493}{2213042} & \frac{3977337}{1008884} & \frac{336842}{950879} & \frac{-10931975}{737743} & \frac{-586849}{397609} \\ \frac{-672384}{487907} & \frac{6197680}{1485339} & \frac{290655}{775219} & \frac{-17268043}{1101025} & \frac{-1015105}{649813} \end{array} \right],$$

$$B = \left[\begin{array}{ccccc} \frac{5108949}{822212} & \frac{-9636557}{3096360} & \frac{17025}{771748} & \frac{289432}{533353} & \frac{-110837}{809445} \\ \frac{18550547}{1412647} & \frac{-7713256}{1222519} & \frac{-132617}{2924009} & \frac{2955541}{2513118} & \frac{-273787}{931060} \\ \frac{12234958}{608309} & \frac{-14462842}{1492679} & \frac{39199}{284488} & \frac{1104843}{627526} & \frac{-298985}{673039} \\ \frac{18054598}{768283} & \frac{-6743249}{591029} & \frac{342131}{1110339} & \frac{1953199}{897516} & \frac{-327324}{623023} \\ \frac{67379365}{2710249} & \frac{-17730591}{1470500} & \frac{30199}{136449} & \frac{3382849}{1342415} & \frac{-200585}{428266} \end{array} \right],$$

$$v = \left[\begin{array}{ccccc} \frac{-672384}{487907} & \frac{6197680}{1485339} & \frac{290655}{775219} & \frac{-17268043}{1101025} & \frac{-1015105}{649813} \end{array} \right]^T,$$

$$w = \left[\begin{array}{ccccc} \frac{67379365}{2710249} & \frac{-17730591}{1470500} & \frac{30199}{136449} & \frac{3382849}{1342415} & \frac{-200585}{428266} \end{array} \right]^T.$$

The stability polynomial $p(\omega, z)$ of this method is

$$p(\omega, z) = \omega^5 \Big(\Big(1 - \frac{7}{20}z\Big)^5 - p_1(z)\omega + p_0(z) \Big)$$

with

$$p_1(z) = 1 - \frac{360063}{400000}z + \frac{23017}{400000}z^2 + \frac{68950}{857023}z^3,$$

$$p_0(z) = -\frac{60063}{400000}z - \frac{13523}{200000}z^2.$$

Example 6. TSRK methods with $p = q = s = 6$. The coefficients of the method corresponding to $\lambda = \frac{1}{4}$ and the abscissa vector $c = [0, \frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, 1]^T$ are given by

$$A = \begin{bmatrix} \frac{206761}{486792} & \frac{-2177245}{999613} & \frac{4956617}{1262836} & \frac{-2659937}{1501250} & \frac{-5233080}{1613899} & \frac{-1237915}{1202898} \\ \frac{1221319}{1042825} & \frac{-2334973}{388789} & \frac{2041323}{188617} & \frac{-6575964}{1346011} & \frac{-7149231}{799624} & \frac{-2355280}{830019} \\ \frac{1969593}{895745} & \frac{-8394961}{744520} & \frac{56845577}{2797637} & \frac{-6564097}{715632} & \frac{-298740209}{17796957} & \frac{-2296272}{431017} \\ \frac{5500609}{1789349} & \frac{-13055131}{828162} & \frac{31208158}{1098599} & \frac{-10484818}{817621} & \frac{-40594171}{1729785} & \frac{-6093829}{818159} \\ \frac{2484695}{697381} & \frac{-6233112}{341155} & \frac{47357846}{1438387} & \frac{-11436434}{769475} & \frac{-229860522}{8450951} & \frac{-8605475}{996862} \\ \frac{3494450}{939559} & \frac{-37111484}{1945823} & \frac{31041506}{903181} & \frac{-2953828}{190387} & \frac{-45973675}{1619193} & \frac{-13030852}{1446043} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{12559463}{2371052} & \frac{-304401}{1566979} & \frac{-796357}{279698} & \frac{1215880}{535137} & \frac{-729199}{969976} & \frac{240761}{2509704} \\ \frac{13632701}{929185} & \frac{-398936}{1182213} & \frac{-14663406}{1841771} & \frac{5592299}{883194} & \frac{-2074575}{989342} & \frac{67223}{250581} \\ \frac{21218618}{772033} & \frac{-532052}{739999} & \frac{-10418382}{708325} & \frac{6260019}{530806} & \frac{-4109866}{1052423} & \frac{1009813}{2024284} \\ \frac{48917180}{1273853} & \frac{-2232926}{1972181} & \frac{-6614283}{323212} & \frac{21956107}{1323707} & \frac{-5219169}{954631} & \frac{570709}{817563} \\ \frac{76962919}{1729681} & \frac{-849049}{631226} & \frac{-21833631}{918277} & \frac{35687693}{1844936} & \frac{-6549440}{1048933} & \frac{540181}{671271} \\ \frac{37000571}{796584} & \frac{-861014}{597671} & \frac{-28722443}{1160134} & \frac{8314220}{414279} & \frac{-4232029}{669366} & \frac{109037}{120350} \end{bmatrix},$$

$$v = \begin{bmatrix} \frac{3494450}{939559} & \frac{-37111484}{1945823} & \frac{31041506}{903181} & \frac{-2953828}{190387} & \frac{-45973675}{1619193} & \frac{-13030852}{1446043} \end{bmatrix}^T,$$

$$w = \begin{bmatrix} \frac{37000571}{796584} & \frac{-861014}{597671} & \frac{-28722443}{1160134} & \frac{8314220}{414279} & \frac{-4232029}{669366} & \frac{109037}{120350} \end{bmatrix}^T.$$

The stability polynomial $p(\omega, z)$ of this method is

$$p(\omega, z) = \omega^6\Big(\Big(1 - \frac{1}{4}z\Big)^6 - p_1(z)\omega + p_0(z)\Big)$$

with

$$p_1(z) = 1 - \frac{947389}{1060975}z + \frac{175073}{1568033}z^2 + \frac{5749}{216200}z^3,$$

$$p_0(z) = -\frac{318846}{811433}z - \frac{218512}{998727}z^2 - \frac{16078}{429949}z^3.$$

Example 7. TSRK methods with $p = q = s = 7$. The coefficients of the method corresponding to $\lambda = \frac{13}{50}$ and the abscissa vector $c = [0, \frac{1}{6}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, \frac{5}{6}, 1]^T$ are given by

$$A = \begin{bmatrix} \frac{1783335}{676924} & \frac{-7538683}{457692} & \frac{43678077}{1049267} & \frac{-54284841}{1022633} & \frac{33777979}{937657} & \frac{-7198262}{356705} & \frac{379683}{1080112} \\ \frac{3729799}{735908} & \frac{-20367633}{642761} & \frac{72355517}{903494} & \frac{-82333052}{806207} & \frac{71311153}{1028961} & \frac{-59002918}{1519799} & \frac{725528}{1072835} \\ \frac{5991341}{863556} & \frac{-14152977}{326276} & \frac{67851404}{618929} & \frac{-130388531}{932696} & \frac{76757929}{809083} & \frac{-56042180}{1054523} & \frac{424213}{458238} \\ \frac{6715081}{877512} & \frac{-228392010}{4773683} & \frac{144600295}{1195877} & \frac{-148311987}{961861} & \frac{108811375}{1039871} & \frac{-38121276}{650345} & \frac{1152775}{1128982} \\ \frac{5598709}{726350} & \frac{-33826821}{701924} & \frac{152607948}{1252999} & \frac{-103762415}{668086} & \frac{171340501}{1625629} & \frac{-76481641}{1295358} & \frac{437020}{424913} \\ \frac{16839303}{2218079} & \frac{-24069939}{507106} & \frac{112928115}{941392} & \frac{-172616717}{1128418} & \frac{184411781}{1776417} & \frac{-64700798}{1112595} & \frac{1357207}{1339799} \\ \frac{17189707}{2289435} & \frac{-51762970}{1102681} & \frac{103097327}{869006} & \frac{-614615108}{4062537} & \frac{230612016}{2246183} & \frac{-54870913}{954062} & \frac{695949}{694669} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{34603261}{1388554} & \frac{-19233572}{815029} & \frac{2030231}{1173350} & \frac{22887644}{1581295} & \frac{-18435947}{1539801} & \frac{2486545}{609454} & \frac{-287001}{535772} \\ \frac{52352438}{1090781} & \frac{-62923957}{1391490} & \frac{3783300}{1182001} & \frac{20813831}{744708} & \frac{-24191511}{1047718} & \frac{13984141}{1777666} & \frac{-885477}{857243} \\ \frac{94431588}{1437773} & \frac{-32965493}{532566} & \frac{6732933}{1477091} & \frac{18746689}{491054} & \frac{-18453504}{584585} & \frac{14100872}{1310931} & \frac{-1490328}{1055203} \\ \frac{39601297}{546694} & \frac{-29597137}{433299} & \frac{2472715}{483671} & \frac{37107199}{879216} & \frac{-18665405}{535864} & \frac{11132654}{938101} & \frac{-281828}{180873} \\ \frac{67418527}{924008} & \frac{-89376929}{1299082} & \frac{4456711}{868713} & \frac{86203912}{2022917} & \frac{-31715717}{906161} & \frac{9266149}{775688} & \frac{-2079903}{1325867} \\ \frac{59500172}{827943} & \frac{-264345204}{3900895} & \frac{5409897}{1066186} & \frac{565393}{13484} & \frac{-31677679}{922400} & \frac{8211829}{693856} & \frac{-1877703}{1213402} \\ \frac{52093647}{732968} & \frac{-43427686}{648181} & \frac{2907703}{585819} & \frac{44100315}{1060744} & \frac{-32146509}{942964} & \frac{10865491}{914213} & \frac{-11407715}{7718976} \end{bmatrix},$$

$$v = \begin{bmatrix} \frac{17189707}{2289435} & \frac{-51762970}{1102681} & \frac{103097327}{869006} & \frac{-614615108}{4062537} & \frac{230612016}{2246183} & \frac{-54870913}{954062} & \frac{695949}{694669} \end{bmatrix}^T,$$

$$w = \begin{bmatrix} \frac{52093647}{732968} & \frac{-43427686}{648181} & \frac{2907703}{585819} & \frac{44100315}{1060744} & \frac{-32146509}{942964} & \frac{10865491}{914213} & \frac{-11407715}{7718976} \end{bmatrix}^T.$$

The stability polynomial $p(\omega, z)$ of this method is

$$p(\omega, z) = \omega^7 \Big(\Big(1 - \frac{13}{50} z \Big)^7 - p_1(z)\omega + p_0(z) \Big)$$

with

$$p_1(z) = 1 - \frac{416477}{1583260} z - \frac{229249}{721861} z^2 + \frac{305139}{1474364} z^3 - \frac{48467}{1303694} z^4,$$

$$p_0(z) = \frac{348665}{626026} z + \frac{146321}{1046876} z^2 + \frac{8403}{1175114} z^3.$$

Example 8. TSRK methods with $p = q = s = 8$. The coefficients of the method corresponding to $\lambda = \frac{1}{5}$ and the abscissa vector $c = [0, \frac{1}{7}, \frac{2}{7}, \frac{3}{7}, \frac{4}{7}, \frac{5}{7}, \frac{6}{7}, 1]^T$

are given by

$$A = \begin{bmatrix} \frac{-714138}{227233} & \frac{34790019}{1392476} & \frac{-53301137}{628189} & \frac{167294409}{1060088} & \frac{-306224974}{1805161} & \frac{60624942}{598429} & \frac{-31988668}{916041} & \frac{2680603}{438798} \\ \frac{-2416325}{511814} & \frac{152422532}{4061157} & \frac{-75464143}{592055} & \frac{306391443}{1292423} & \frac{-238452872}{935719} & \frac{131985577}{867272} & \frac{-50292551}{958716} & \frac{11349405}{1236724} \\ \frac{-10251917}{1509329} & \frac{8135387}{150661} & \frac{-182141731}{993237} & \frac{354764764}{1040137} & \frac{-249438226}{680343} & \frac{164398219}{750841} & \frac{-59165330}{783927} & \frac{26279871}{1990421} \\ \frac{-10589606}{1236985} & \frac{35206127}{517305} & \frac{-162887481}{704753} & \frac{267548092}{622383} & \frac{-139563607}{302025} & \frac{345701691}{1252732} & \frac{-137870526}{1449391} & \frac{22369407}{1344256} \\ \frac{-11544228}{1149833} & \frac{11492131}{143984} & \frac{-441900815}{1630269} & \frac{287646235}{570558} & \frac{-574398702}{1059911} & \frac{44449916}{137345} & \frac{-447058553}{4007410} & \frac{13920551}{713295} \\ \frac{-3013026}{265405} & \frac{163431069}{1810859} & \frac{-196745135}{641911} & \frac{495505820}{869213} & \frac{-470948712}{768539} & \frac{390310186}{1066567} & \frac{-146881795}{1164404} & \frac{22707495}{1029007} \\ \frac{-5121537}{408010} & \frac{90577214}{907681} & \frac{-477042901}{1407643} & \frac{687350054}{1090485} & \frac{-538544390}{794837} & \frac{486019835}{1201148} & \frac{-271627329}{1947482} & \frac{27007063}{1106855} \\ \frac{-16048057}{1189994} & \frac{119831339}{1117729} & \frac{-132088075}{362786} & \frac{325044759}{479995} & \frac{-463100999}{636186} & \frac{329337818}{757593} & \frac{-101397601}{676674} & \frac{20020383}{763726} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{5065317}{278834} & \frac{-15365130}{703469} & \frac{-11135701}{1048147} & \frac{26469955}{671091} & \frac{-26922302}{755283} & \frac{16232681}{987854} & \frac{-7401603}{1847926} & \frac{192469}{464674} \\ \frac{38506450}{1408799} & \frac{-47461928}{1453829} & \frac{-20226373}{1256011} & \frac{79490963}{1338286} & \frac{-53022378}{988273} & \frac{25566519}{1033666} & \frac{-5369003}{890335} & \frac{671288}{1076049} \\ \frac{94806865}{2412159} & \frac{-90195025}{1919661} & \frac{-26647373}{1159290} & \frac{80004065}{937473} & \frac{-74345674}{964123} & \frac{41705227}{1173141} & \frac{-4752779}{548405} & \frac{841048}{938235} \\ \frac{8076507}{163075} & \frac{-19188129}{323684} & \frac{-36904738}{1277149} & \frac{67033053}{622801} & \frac{-98205601}{1010408} & \frac{80147498}{1788801} & \frac{-12867653}{1178095} & \frac{184748}{163535} \\ \frac{26318004}{453167} & \frac{-50775833}{729980} & \frac{-33037981}{974354} & \frac{128494339}{1017570} & \frac{-32228512}{282981} & \frac{66883087}{1273296} & \frac{-36423076}{2844381} & \frac{1738343}{1312523} \\ \frac{49284925}{750569} & \frac{-60342586}{766911} & \frac{-45712898}{1192413} & \frac{212349752}{1487813} & \frac{-65561113}{509486} & \frac{58350037}{981351} & \frac{-15250587}{1052989} & \frac{362983}{242337} \\ \frac{113267199}{1560178} & \frac{-74577173}{857027} & \frac{-47044078}{1109361} & \frac{235718822}{1493617} & \frac{-133917767}{940808} & \frac{72166703}{1095884} & \frac{-20375991}{1277015} & \frac{803050}{485413} \\ \frac{46503998}{596239} & \frac{-98294310}{1051067} & \frac{-55888789}{1227983} & \frac{1581139891}{9332284} & \frac{-605910987}{3965800} & \frac{38271901}{542181} & \frac{-13717940}{807873} & \frac{1586639}{871379} \end{bmatrix},$$

$$v = \begin{bmatrix} \frac{-16048057}{1189994} & \frac{119831339}{1117729} & \frac{-132088075}{362786} & \frac{325044759}{479995} & \frac{-463100999}{636186} & \frac{329337818}{757593} & \frac{-101397601}{676674} & \frac{20020383}{763726} \end{bmatrix}^T,$$

$$w = \begin{bmatrix} \frac{46503998}{596239} & \frac{-98294310}{1051067} & \frac{-55888789}{1227983} & \frac{1581139891}{9332284} & \frac{-605910987}{3965800} & \frac{38271901}{542181} & \frac{-13717940}{807873} & \frac{1586639}{871379} \end{bmatrix}^T.$$

The stability polynomial $p(\omega, z)$ of this method is

$$p(\omega, z) = \omega^8 \left(\left(1 - \frac{1}{5}z\right)^8 - p_1(z)\omega + p_0(z) \right)$$

with

$$p_1(z) = 1 + \frac{7274497}{6752382}z - \frac{699451}{758229}z^2 + \frac{122005}{454009}z^3 - \frac{37033}{1217147}z^4,$$

$$p_0(z) = \frac{2266669}{1351361}z + \frac{852169}{1159661}z^2 + \frac{124134}{983293}z^3 + \frac{10532}{1176849}z^4.$$

8 Numerical experiments

In this section we will demonstrate that the TSRK methods of order p and stage order $q = p$ do not suffer from order reduction which is the case for classical Runge-Kutta formulas. To illustrate this we have applied the Runge-Kutta-Gauss method of order $p = 4$ and stage order $q = 2$ and TSRK method of order $p = 4$ and stage order $q = 4$ given in Example 4 in Section 7 to the van der Pol oscillator (see VDPOL problem in [22])

$$\begin{cases} y_1' = y_2, & y_1(0) = 2, \\ y_2' = \big((1 - y_1^2)y_2 - y_1\big)/\epsilon, & y_2(0) = -2/3, \end{cases} \tag{8.1}$$

$t \in [0, T]$, with a stiffness parameter ϵ. We have implemented both methods with a fixed stepsize $h = T/N$, and observed the order of convergence of numerical approximations to the slowly varying parts of the solution, where the problem is stiff for small values of the parameter ϵ (the problem is not stiff on the interval where the solution is changing rapidly). Similarly as in [22], in order to reduce the influence of round-off errors the TSRK methods (1.4) (with $\theta = 0$ and $u = 0$) were rewritten in the form

$$\left\{\begin{array}{lcl} Z^{[n]} & = & h(A \otimes I_m)f(Z^{[n-1]} + (e \otimes I_m)y_{n-2}) \\ & + & h(B \otimes I_m)f(Z^{[n]} + (e \otimes I_m)y_{n-1}), \\ y_n & = & y_{n-1} + h(v^T \otimes I_m)f(Z^{[n-1]} + (e \otimes I_m)y_{n-2}) \\ & + & h(w^T \otimes I_m)f(Z^{[n]} + (e \otimes I_m)y_{n-1}), \end{array}\right. \tag{8.2}$$

$n = 2, 3, \ldots, N$, where

$$Z^{[n]} := Y^{[n]} - (e \otimes I_m)y_{n-1}$$

is usually smaller than $Y^{[n]}$. Define

$$\begin{array}{lcl} G(Z^{[n]}) & := & Z^{[n]} - h(A \otimes I_m)f(Z^{[n-1]} + (e \otimes I_m)y_{n-2}) \\ & - & h(B \otimes I_m)f(Z^{[n]} + (e \otimes I_m)y_{n-1}), \end{array}$$

and denote by $J = J(y_{n-1})$ the Jacobian of the right hand side of (8.1) computed at y_{n-1}. Then similarly as in [22] an approximation to $Z^{[n]}$ is computed by simplified Newton iterations

$$\begin{cases} \big(I - h(B \otimes J)\big)\Delta Z_k^{[n]} = -G(Z_k^{[n]}), \quad k = 0, 1, 2, \ldots, \\ Z_{k+1}^{[n]} = Z_k^{[n]} + \Delta Z_k^{[n]}, \end{cases}$$

with $Z_0^{[n]} = 0$ and a stopping criterion similar to that used in [22] in case of Runge-Kutta methods.

N	$\epsilon = 10^{-1}$		$\epsilon = 10^{-3}$		$\epsilon = 10^{-6}$	
	$\Vert e_h^{RKG}(T)\Vert$	p	$\Vert e_h^{RKG}(T)\Vert$	p	$\Vert e_h^{RKG}(T)\Vert$	p
32	$3.02 \cdot 10^{-7}$		$2.19 \cdot 10^{-3}$		$5.83 \cdot 10^{-3}$	
64	$1.88 \cdot 10^{-8}$	4.00	$2.25 \cdot 10^{-4}$	3.28	$1.49 \cdot 10^{-3}$	1.97
128	$1.18 \cdot 10^{-9}$	4.00	$1.68 \cdot 10^{-5}$	3.74	$3.71 \cdot 10^{-4}$	2.01
256	$8.21 \cdot 10^{-11}$	3.84	$1.11 \cdot 10^{-6}$	3.93	$8.84 \cdot 10^{-5}$	2.07
512	$1.43 \cdot 10^{-11}$	2.52	$7.02 \cdot 10^{-8}$	3.98	$1.87 \cdot 10^{-5}$	2.24

Table 8.1: Numerical results for Runge-Kutta-Gauss method of order $p = 4$ and stage order $q = 2$

The results of numerical experiments for fixed stepsize implementations of Runge-Kutta-Gauss method of order $p = 4$ and stage order $q = 2$ and TSRK method (8.2) of order $p = 4$ and stage order $q = 4$ given in Example 4 in Section 7 are presented in Table 1 and Table 2, respectively. These results correspond to $T = 2/3$, $h = T/N$, and $N = 32$, 64, 128, 256 and 512. In these tables we have listed norms of errors $\Vert e_h^{RKG}(T)\Vert$ and $\Vert e_h^{TSRK}(T)\Vert$ at the endpoint of integration T and the observed order of convergence p computed from the formula

$$p = \frac{\log\left(\Vert e_h(T)\Vert / \Vert e_{h/2}(T)\Vert\right)}{\log(2)},$$

where $e_h(T)$ and $e_{h/2}(T)$ are errors corresponding to stepsizes h and $h/2$ for Runge-Kutta-Gauss and TSRK methods. We can observe that for the values of $\epsilon = 10^{-1}$ and $\epsilon = 10^{-3}$ for which the problem (8.1) is not stiff and mildly stiff both methods are convergent with expected order $p = 4$ (although there is an unexpected reduction to order $p = 2.52$ only for Runge-Kutta method for $N = 512$). However, for small values of ϵ ($\epsilon = 10^{-6}$) for which the van der Pol oscillator (8.1) is stiff the Runge-Kutta Gauss method exhibits order reduction phenomenon and its order of convergence drops to about $p = 2$ which corresponds to the stage order $q = 2$. This is not the case for TSRK method which preserves order of convergence $p = q = 4$, which leads to higher accuracy.

We also present in Fig. 5 the comparison of fixed stepsize implementations of SDIRK method of order $p = 3$ and stage order $q = 2$ (see [9], p. 234) and TSRK method of order $p = 3$ and stage order $q = 3$ given in Example 3 in Section 7. These results correspond to $T = 3/4$ and $\epsilon = 10^{-4}$. We can see again that in contrast to SDIRK formula TSRK method does

N	$\epsilon = 10^{-1}$		$\epsilon = 10^{-3}$		$\epsilon = 10^{-6}$	
	$\|e_h^{TSRK}(T)\|$	p	$\|e_h^{TSRK}(T)\|$	p	$\|e_h^{TSRK}(T)\|$	p
32	$7.83 \cdot 10^{-7}$		$1.85 \cdot 10^{-4}$		$2.44 \cdot 10^{-4}$	
64	$1.03 \cdot 10^{-7}$	2.93	$1.94 \cdot 10^{-5}$	3.25	$2.65 \cdot 10^{-5}$	3.21
128	$7.67 \cdot 10^{-9}$	3.75	$1.57 \cdot 10^{-6}$	3.62	$2.20 \cdot 10^{-6}$	3.59
256	$5.17 \cdot 10^{-10}$	3.89	$1.09 \cdot 10^{-7}$	3.85	$1.59 \cdot 10^{-7}$	3.79
512	$4.21 \cdot 10^{-11}$	3.62	$6.52 \cdot 10^{-9}$	4.06	$1.08 \cdot 10^{-8}$	3.89

Table 8.2: Numerical results for TSRK method of order $p = 4$ and stage order $q = 4$

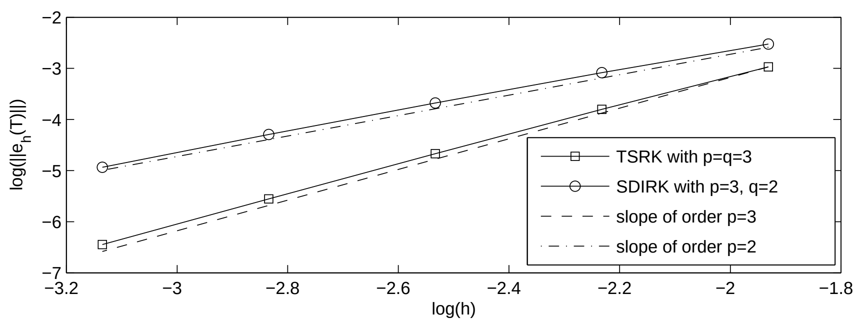

Figure 5: Numerical results for SDIRK formula with $p = 3$ and $q = 2$ and TSRK method with $p = q = 3$ on the problem (8.1) with $\epsilon = 10^{-4}$

not suffer from order reduction phenomenon. Additional results which confirm that TSRK methods constructed in this paper preserve the order of convergence for stiff problems are given in [18].

9 Concluding remarks and future work

We described the construction of highly stable TSRK methods with IQS properties, i.e., methods for which stability properties are determined by quadratic stability polynomials. We also imposed the condition that the coefficient matrix B has a one point spectrum $\sigma(B) = \{\lambda\}$, $\lambda > 0$, which facilitates the efficient implementation of these methods similarly as in the case of SIRK methods. The interest in IQS property lies in its ability to handle the problem of deriving A-stable, L-stable, and possibly algebraically stable TSRK methods, and also succeeding in managing the computations in a symbolic environment for large number of stages s. The methods which were derived have uniform order $p = q = s$, where s is the number of stages. Examples of methods are presented up to the order eight. These methods do not suffer from the order reduction phenomenon (see [9, 11, 22]), which usually occurs in the numerical integration of stiff problems by Runge-Kutta formulas.

The implementation issues related to these methods and comparisons with other methods are the subject of current work and will be reported elsewhere. They include the choice of appropriate starting procedures, estimation of local discretization errors for small and large stepsizes, filtering error estimates for stiff problems, construction of continuous interpolants, design of stepsize and order changing strategies, and strategies for efficient solution of system of nonlinear equations which take advantage of one point spectrum of the coefficient matrix B. All these implementation issues were already investigated in the context of two step almost collocation methods in the recent paper [20]. It is hoped that this work, which is also described in the Ph.D. thesis of the second author [18], will lead to efficient variable-stepsize variable-order algorithms for the numerical solution of stiff systems of ODEs.

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