SYMPLECTIC RUNGE-KUTTA SCHEMES II: CLASSIFICATION OF SYMMETRIC METHODS

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Abstract. A complete classification of all symplectic self-adjoint Runge-Kutta methods with up to 6 stages is given and the derivation process used is outlined. This is made possible by the fact that most of these schemes are determined by *linear* systems of simplifying equations. Furthermore, the derivation process can be used for higher stage numbers but not without loss of generality. We also show how it is often straightforward to derive subclasses of methods possessing additional desirable properties, such as algebraic stability. Extensive use of computer algebra has proven invaluable in the classification process.

Key words. Runge-Kutta, order conditions, symplectic, symmetric, self-adjoint, Hamiltonian systems, canonical, symplectic integration

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Contents

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1 Introduction

In recent years there have been numerous articles justifying the qualitative advantages of using symplectic integrators for Hamiltonian systems [14]. There have also been advances in establishing the conditions that established numerical schemes, such as Runge-Kutta methods, must satisfy in order to be symplectic. However, despite these advances, there has been very little work done to apply these theoretical frameworks to the systematic construction of practical methods. Much of the work that has been carried out on the construction of Runge-Kutta schemes, has been of a heuristic nature, often utilizing numerical minimization codes (see [11, 3] for some examples in the context of symplectic methods). That is, any freedom in the choice of schemes is eliminated by restricting attention to specific methods often using some subsidiary constraints, such as minimizing principal error coefficients. Others have used established tools such as perturbed collocation and W-transforms to illustrate how particular symplectic methods can be constructed [7, 8].

There are obvious problems with these approaches. Any classification of methods forms only a subset of those possible. Furthermore failure to find methods of a specific class contributes no information to address the important question of existence.

The primary goal of this work is to provide a comprehensive study of a class of symplectic Runge-Kutta schemes which possess a certain symmetry. This symmetry helps to further reduce the number of constraints which must be considered by eliminating all even order conditions. Furthermore it has been shown that methods possessing this symmetry possess desirable properties in their own right (see for example [2] and the references therein).

Another benefit of our approach is that, since we are always working with the most general solutions, we are able to impose additional algebraic constraints in a simple manner. This allows us to build upon our results for symplectic methods and use them to construct additional classes of methods. For example, all symplectic schemes with positive weights satisfy the desirable property of algebraic stability for dissipative systems.

Here we will present a complete categorization of all symplectic symmetric (self-adjoint) schemes through $s = 6$ stages. These encompass the familiar Gauss-Legendre methods whose order is twice the stage number. We will demonstrate that the reason that this task can be accomplished, is because the categorization is tantamount to merely solving quadrature conditions in conjunction with *linear* systems of equations: the simplifying assumptions.

The final construction which we present here hides the often twisted path by which our results were obtained. Indeed we have used computer algebra extensively to automate the formalism of Butcher [15] and that of symplectic Runge-Kutta methods [16]. This has facilitated tremendously in the formation and verification of conjectures at various stages of this work. We used two computer algebra systems, MAPLE [4] and MATHEMATICA [19], to confirm the results presented here independently, in order to minimize errors which might be present in either system, human error, and to minimize transcription errors in the text of this article.

The paper is organized as follows: In section 2 we review some elements of Runge-Kutta theory. In particular, in subsection 2.2 Butcher's theory of order and its symplectic modification, developed in [16], are summarized. In subsection 2.3 we review the role of simplifying assumptions. We show that for stage numbers $s \leq 6$ the simplifying assumptions are necessarily satisfied for most self-adjoint schemes. In section 3 a complete list of multi-parameter families of self-adjoint symplectic schemes is derived, where self-adjointness is induced by a "standard" symmetry structure in the Butcher parameters. These results encompass methods through 6 stages and order 12. They are derived using symbolic computation, solving non-linear quadrature conditions together with the linear equations arising from simplifying assumptions. In section 4 methods with "non-standard" symmetry structure are considered and categorized through 6 stages. In section 5 we comment on a subclass of algebraically stable Runge-Kutta methods, which are given by the symplectic schemes of the previous sections with positive weights. The appendix reviews some results from the representation theory of permutation groups used in section 4.

2 Theoretical background

2.1 Self-adjoint and symplectic Runge-Kutta schemes

Given an initial value problem for a system of first order differential equations:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(t, \mathbf{y}), \qquad \mathbf{y}(t_0) = \mathbf{y}_0 \,.$$

A Runge-Kutta method with s stages for this system is given by the map $\Psi_h : \mathbf{y}_n \mapsto \mathbf{y}_{n+1}$:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{j=1}^{s} b_j \, \mathbf{f}(t_n + c_j \, h, \mathbf{y}^{(j)}) \ ,$$

where the *internal stages* $\mathbf{y}^{(j)}$ are the solutions of the following non-linear system of algebraic equations

$$\mathbf{y}^{(i)} = \mathbf{y}_n + h \sum_{j=1}^{s} a_{ij} \, \mathbf{f}(t_n + c_j h, \mathbf{y}^{(j)}) \ , \quad i = 1, \ldots, s. \tag{2.1}$$

The parameters c_j, b_j and a_{ij} have to be chosen such that $\mathbf{y}_n$ represents an approximation of the Taylor expansion of the solution. The coefficients c_i are given by the row-sum conditions:

$$c_i = \sum_{j=1}^{s} a_{ij} \ , \quad i = 1, \dots, s \ . \tag{2.2}$$

It has become customary to represent the free parameters of the method using a *Butcher tableau* [1]:

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

A Runge-Kutta method is said to be *irreducible* [5], if $b_j \neq 0$, $j = 1, \dots, s$. We shall assume irreducibility throughout this paper. Without loss of generality we may rewrite the Butcher tableau in terms of new parameters $\tilde{c}_i$ and s_{ij} given by

$$c_i \ = \ \frac{1}{2} + \tilde{c}_i \ , \quad a_{ij} \ = \ \left(\frac{1}{2} + s_{ij}\right) b_j \ , \quad i, j = 1, \dots, s \ ,$$

where the modified row sums satisfy

$$\tilde{c}_i = \sum_{j=1}^{s} s_{ij} \, b_j \tag{2.3}$$

under the consistency assumption $\sum_j b_j = 1$. In the following we shall use the matrix $S = (s_{ij})$ and the column vectors $\tilde{\mathbf{c}} = (\tilde{c}_1, \dots, \tilde{c}_s)^T$, $\mathbf{b} = (b_1, \dots, b_s)^T$ to denote the Butcher parameters.

We note that the Runge-Kutta map $\Psi_h : \mathbf{y}_n \mapsto \mathbf{y}_{n+1}$ is characterized by these parameters only up to permutation of the internal stages:

Definition 2.1 *Two sets of Butcher parameters $S, \tilde{\mathbf{c}}, \mathbf{b}$ and $S', \tilde{\mathbf{c}}', \mathbf{b}'$ are called* **equivalent**, *if*

$$S' = \mathcal{P} S \mathcal{P}^{-1} \ , \quad \tilde{\mathbf{c}}' = \mathcal{P} \tilde{\mathbf{c}} \ , \quad \mathbf{b}' = \mathcal{P} \mathbf{b}$$

with some permutation matrix[1] $\mathcal{P}$*, i.e.,*

$$s'_{ij} = s_{\sigma(i),\sigma(j)} \ , \quad \tilde{c}'_i = \tilde{c}_{\sigma(i)} \ , \quad b'_i = b_{\sigma(i)} \ , \quad i, j = 1, \dots, s$$

with some permutation $\sigma : \{1, \dots, s\} \mapsto \{1, \dots, s\}$.

Equivalent sets of parameters generate the same map Ψ_h. Further, some of the internal stages $\mathbf{y}^{(i)}$ in (2.1) may coincide. In this case the scheme reduces to one with less stages:

[1]For a permutation σ the corresponding permutation matrix $\mathcal{P}(\sigma)$ is given by $(\mathcal{P}(\sigma))_{ij} = 1$ for $i = \sigma(j)$ and $(\mathcal{P}(\sigma))_{ij} = 0$ for $i \neq \sigma(j)$. This is the usual matrix representation of the symmetric group: $\mathcal{P}(\sigma_1 \circ \sigma_2) = \mathcal{P}(\sigma_1)\mathcal{P}(\sigma_2)$.

Remark 2.2 *If two rows j_1 and j_2, say, coincide in S, then $\mathbf{y}^{(j_1)} = \mathbf{y}^{(j_2)}$ in (2.1) and the method reduces to a scheme with $s-1$ stages. Combining the internal stages $\mathbf{y}^{(j_1)}$ and $\mathbf{y}^{(j_2)}$ the parameters $S', \tilde{\mathbf{c}}', \mathbf{b}'$ of the reduced method are obtained by deleting the row and the column j_2 from the Butcher tableau and replacing the column j_1 by the sum of the original columns j_1 and j_2:*

$$s'_{ij_1} b'_{j_1} = s_{ij_1} b_{j_1} + s_{ij_2} b_{j_2} \ , \quad i \in \{1, \ldots, s\} \setminus \{j_2\} \ , \quad \tilde{c}'_{j_1} = \tilde{c}_{j_1} \ , \quad b'_{j_1} = b_{j_1} + b_{j_2} \ .$$

Following [16] *self-adjoint (symmetric)* schemes are characterized by the constraints $S = -\mathcal{P} S \mathcal{P}^{-1}$, $\tilde{\mathbf{c}} = -\mathcal{P}\tilde{\mathbf{c}}$, $\mathbf{b} = \mathcal{P}\mathbf{b}$ with some permutation matrix $\mathcal{P}$, i.e.,

$$s_{ij} = -s_{\sigma(i),\sigma(j)} \ , \quad \tilde{c}_i = -\tilde{c}_{\sigma(i)} \ , \quad b_i = b_{\sigma(i)} \ , \quad i, j = 1, \ldots, s \tag{2.4}$$

with some permutation $\sigma : \{1, \ldots, s\} \mapsto \{1, \ldots, s\}$. These methods provide their own inverse upon time reversal: $\Psi_{-h} = \Psi_h^{-1}$. The symmetry structure (2.4) provides a set of linear constraints on the Runge-Kutta method. They ensure that all the even order terms in the local error expansion are satisfied.

A simple algebraic relation ensuring that a Runge-Kutta method is symplectic has been shown to be [9, 13, 18]:

$$b_i \, a_{ij} + b_j \, a_{ji} - b_i \, b_j = 0 \ , \quad i, j = 1, \ldots, s \ . \tag{2.5}$$

This condition has also been shown to be necessary for irreducible schemes [14]. In terms of the new parameters $S = (s_{ij})$ symplecticity amounts to skew-symmetry of S:

$$s_{ij} = -s_{ji} \ , \quad i, j = 1, \ldots, s \ . \tag{2.6}$$

We note that the assumption of irreducibility $b_j \neq 0$ is very natural in the symplectic context: if $b_{j_0} = 0$, then (2.5) implies $a_{ij_0} = 0$ for any stage i with non-trivial weight b_i. Consequently, the stage j_0 does not contribute to the Runge-Kutta map Ψ_h and the scheme reduces to one with $s-1$ stages.

The symplecticity condition represents additional linear constraints on the free parameters which must be satisfied in conjunction with the order conditions. Although at first it may seem that for a given number of parameters some order equations have to be sacrificed in favor of symplecticity, it turns out that a considerable number of the order conditions become dependent. Thus, the constraints imposed by symplecticity do not lead to order barriers but rather serve as simplifying assumptions.

In this article we shall be concerned with the class of Runge-Kutta methods which are both symplectic and self-adjoint. The richest family of schemes arises from self-adjointness induced by the permutation $\sigma(i) = s + 1 - i$, which shall be referred to as the "standard" case. The constraints (2.4) and (2.6) lead to Butcher parameters of the form

$$S = \begin{pmatrix} 0 & s_{12} & s_{13} & \cdots & \cdots & \\ -s_{12} & 0 & s_{23} & \cdots & & \cdots \\ -s_{13} & -s_{23} & \ddots & & \cdots & \cdots \\ \cdots & \cdots & & \ddots & s_{23} & s_{13} \\ \cdots & & \cdots & -s_{23} & 0 & s_{12} \\ & \cdots & \cdots & -s_{13} & -s_{12} & 0 \end{pmatrix}, \tag{2.7}$$

$$\tilde{\mathbf{c}} = (\tilde{c}_1, \tilde{c}_2, \ldots, -\tilde{c}_2, -\tilde{c}_1)^T , \quad \mathbf{b} = (b_1, b_2, \ldots, b_2, b_1)^T .$$

This parametrization reduces the parameter space without the need to impose side conditions. It has the desirable property that order conditions arising from root isomorphic trees become equivalent due to symplecticity and lower order dependencies are filtered out. Further, all order equations associated with even trees are satisfied automatically due to self-adjointness.

This formalism has the immediate advantage that desirable structural properties result in a reduction of the parameter space and a reduction in the number of terms occurring in the order conditions.[2] This has the benefit of reducing execution time and memory requirements in a computer based implementation of the formalism. The result is a reduction in intermediary expression swell, such a prevalent concern in computer algebra, when performing subsequent symbolic manipulation and solving systems of equations.

2.2 Order conditions

Following Butcher [1, section 35] a Runge-Kutta scheme is said to be of order p, if and only if the *order conditions*

$$\Phi(t) = \frac{1}{\gamma(t)}$$

are satisfied for all rooted trees t through p vertices. For a tree with n vertices, the *weight* Φ, a polynomial in the Butcher parameters, is defined via a labeled representative $t = [(V, E, r)]$:

$$\Phi(t) = \sum_{j_1=1}^{s} \cdots \sum_{j_n=1}^{s} b_{j_r} \prod_{(i,k)\in E} a_{j_i j_k} .$$

Here $V = \{1, \ldots, n\}$ is the index set for the vertices, $E \subset V \times V$ is the set of edges and $r \in V$ is the label of the root. The *density* γ is a combinatorial quantity, i.e., an integer number associated with such a tree [1, definition 144a]. An equivalent set of order conditions, more suitable for self-adjoint and symplectic schemes, was derived in [16]:

$$\tilde{\Phi}(t) = \tilde{\delta}(t)$$

[2] The number of free parameters is just $\lfloor (s+1)^2/4 \rfloor$ where $\lfloor x \rfloor$, $x \in \mathbb{Q}$ denotes the integer part of x [16].

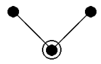
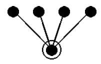
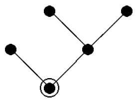
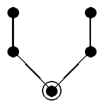
order	t	graph	$\tilde{\Phi}(t) = \tilde{\delta}(t)$
1	τ		$\sum_i b_i = 1$
3	$[\tau^2]$		$\sum_i b_i \, \tilde{c}_i^2 = \frac{1}{12}$
5	$[\tau^4]$		$\sum_i b_i \, \tilde{c}_i^4 = \frac{1}{80}$
	$[\tau[\tau^2]]$		$\sum_{ij} b_i \, \tilde{c}_i \, s_{ij} \, b_j \, \tilde{c}_j^2 = \frac{1}{240}$
	$[[\tau]^2]$		$\sum_i b_i \Big(\sum_j s_{ij} \, b_j \, \tilde{c}_j \Big)^2 = \frac{1}{120}$

Table 1: Order conditions for symplectic self-adjoint schemes through order 5 together with the associated rooted trees and their graphs.

for all rooted trees t with up to p vertices. Here

$$\tilde{\Phi}(t) \; = \; \sum_{j_1=1}^{s} \cdots \sum_{j_n=1}^{s} b_{j_r} \prod_{(i,k)\in E} s_{j_i j_k} \, b_{j_k}$$

and $\tilde{\delta}$ is some new combinatorial function on rooted trees. The basic results of [16] are:

i) For self-adjoint schemes satisfying (2.4) with some permutation σ one automatically has $\tilde{\Phi}(t) = \tilde{\delta}(t) = 0$ for all rooted trees t with an even number of vertices.

ii) For symplectic schemes one has $\tilde{\Phi}(t_1) - \tilde{\delta}(t_1) = -\tilde{\Phi}(t_2) + \tilde{\delta}(t_2)$, where t_1 and t_2 are the same trees with the location of their roots one edge apart.

Consequently, for symplectic schemes only one rooted representative per non-rooted tree needs to be considered. For self-adjoint schemes all equations associated with even trees are trivially satisfied. In table 1, the order conditions for symplectic self-adjoint schemes through order 5 together with the associated rooted trees and their graphical representation are given. The root of each tree is encircled.

Of particular interest are the order conditions given by the "bushy" trees $[\tau^{k-1}]$ of height 2. Here we use the notation of [1, section 144]. The equations

$$B(K): \qquad \sum_{j=1}^{s} b_j\, c_j^{k-1} \;=\; \frac{1}{k}\,, \quad k = 1,\dots,K$$

shall be referred to as the *quadrature conditions.* They are equivalent to

$$\tilde{B}(K): \qquad \sum_{j=1}^{s} b_j\, \tilde{c}_j^{k-1} \;=\; \frac{f_k}{k\,2^{k-1}}\,, \quad k = 1,\dots,K$$

with

$$f_k \;=\; \begin{cases} 0 & \text{for even } k\,, \\ 1 & \text{for odd } k\,. \end{cases}$$

They represent the associated order equations through order K:

$$\Phi([\tau^{k-1}]) \;=\; \sum_{j=1}^{s} b_j\, c_j^{k-1}\,, \quad \gamma([\tau^{k-1}]) \;=\; k\,,$$

$$\tilde{\Phi}([\tau^{k-1}]) \;=\; \sum_{j=1}^{s} b_j\, \tilde{c}_j^{k-1}\,, \quad \tilde{\delta}([\tau^{k-1}]) \;=\; \frac{f_k}{k\,2^{k-1}}\,.$$

2.3 Simplifying assumptions

The conditions

$$A(K): \quad A_i^{(k)} = 0\,, \quad i = 1,\dots,s\,, \quad k = 1,\dots,K$$

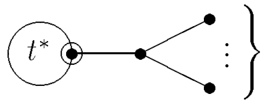
with

$$A_i^{(k)} \;=\; \sum_{j=1}^{s} a_{ij}\, c_j^{k-1} \;-\; \frac{c_i^k}{k}$$

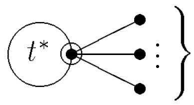
are referred to as the *row simplifying assumptions.* As known from Butcher's work, they lead to dependencies among the order equations associated with different trees. In particular, $A(K)$ implies the relation

$$\Phi(t^{(*,1,k-1)}) \;-\; \frac{1}{\gamma\big(t^{(*,1,k-1)}\big)} \;=\; \frac{1}{k}\left(\Phi(t^{(*,0,k)}) \;-\; \frac{1}{\gamma\big(t^{(*,0,k)}\big)}\right) \tag{2.8}$$

among the order conditions of the trees

$t^{(*,1,k-1)} \;=$ 

$k-1$ terminal vertices

$t^{(*,0,k)} \;=$ 

k terminal vertices,

where the subtree t^* is arbitrary and $k = 1, \ldots, K$. A re-formulation of the row simplifying assumptions involving the new parameters (s_{ij}) is given in [16]. With $c_i = \frac{1}{2} + \tilde{c}_i$ it is easy to verify that the new conditions

$$\tilde{A}(K): \quad \tilde{A}_i^{(k)} = 0 \;, \quad i = 1, \ldots, s \;, \quad k = 1, \ldots, K$$

with

$$\tilde{A}_i^{(k)} \;=\; \sum_{j=1}^{s} s_{ij}\, b_j\, \tilde{c}_j^{\,k-1} \;-\; \frac{\tilde{c}_i^k}{k} \;+\; \frac{f_{k-1}}{k\, 2^k}$$

are equivalent to $A(K)$. The modified simplifying assumptions directly lead to the relations

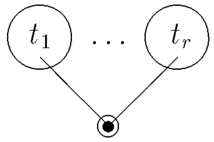
$$\tilde{\Phi}(t^{(*,1,k-1)}) - \tilde{\delta}(t^{(*,1,k-1)}) \;=\; \frac{1}{k}\,\Big(\tilde{\Phi}(t^{(*,0,k)}) - \tilde{\delta}(t^{(*,0,k)})\Big) \;-\; \frac{f_{k-1}}{k\, 2^k}\,\Big(\tilde{\Phi}(t^*) - \tilde{\delta}(t^*)\Big)$$

among the new order equations [16].

Aiming at the construction of Nth order methods, the parameters $\mathbf{b}$, $\tilde{\mathbf{c}}$ are determined by the quadrature conditions $\tilde{B}(N)$. The remaining parameters of the matrix (s_{ij}) then need to be determined by the non-linear order equations. The simplifying assumptions are attractive in that they provide these parameters in terms of $\mathbf{b}$, $\tilde{\mathbf{c}}$ by solving *linear* equations. In particular, one obtains the following statement:

Theorem 2.3 *A symplectic self-adjoint Runge-Kutta method is of order $2n$ if $\tilde{B}(2n-1)$ and $\tilde{A}(n-1)$ hold.*

Proof For self-adjoint schemes the order conditions $\tilde{\Phi}(t) = \tilde{\delta}(t)$ are automatically satisfied for all trees with an even number of vertices. Symplecticity allows to shift the root in any tree without changing the corresponding order equation. Hence only the order conditions of centroids need to be considered. For any tree with an odd number of vertices $2p-1$, $p \le n$, the corresponding centroid has the form



where $r \ge 2$ and each subtree $t_1, \ldots, t_r$ has at most $p - 1 \le n - 1$ vertices. Recursive application of the simplifying principle (2.8) induced by $\tilde{A}(n-1)$ allows to replace all subtrees by "bushy" subtrees with the same number of vertices directly attached to the root. This reduces the tree to the bushy tree $[\tau^{2p-2}]$ for which the order equation is satisfied via the quadrature condition $\tilde{B}(2p-1)$. □

We note that the attribute of self-adjointness may be dropped in theorem 2.3, if $\tilde{B}(2n)$ and $\tilde{A}(n)$ are assumed.

The question arises whether the simplifying assumptions are not just sufficient but also necessary. Firstly, $A(1)$ and $\tilde{A}(1)$ are the row-sum conditions (2.2) and (2.3), which are always assumed. For the higher order assumptions we observe that the quantities $A_i^{(p)}$ and $\tilde{A}_i^{(p)}$ satisfy a set of homogeneous equations induced by the order conditions:

Lemma 2.4 *For any s-stage Runge-Kutta method of order N one has*

$$\sum_{i=1}^{s} b_i\, c_i^{k-1} \left(A_i^{(p)}\right)^m \;=\; \sum_{i=1}^{s} b_i\, \tilde{c}_i^{k-1} \left(\tilde{A}_i^{(p)}\right)^m \;=\; 0$$

for all $k, m, p \in \mathbb{N}$ with $k + mp \leq N$.

Proof Binomial expansion of the expression defining $A_i^{(p)}$ leads to

$$\begin{aligned}
\sum_{i=1}^{s} b_i\, c_i^{k-1} \left(A_i^{(p)}\right)^m &= \sum_{i=1}^{s} b_i\, c_i^{k-1} \sum_{\mu=0}^{m} \binom{m}{\mu} \left(\frac{-c_i^p}{p}\right)^{\mu} \left(\sum_{j=1}^{s} a_{ij}\, c_j^{p-1}\right)^{m-\mu} \\
&= \sum_{\mu=0}^{m} \binom{m}{\mu} \left(\frac{-1}{p}\right)^{\mu} \sum_{i=1}^{s} b_i\, c_i^{k+\mu p-1} \left(\sum_{j=1}^{s} a_{ij}\, c_j^{p-1}\right)^{m-\mu} \\
&= \sum_{\mu=0}^{m} \binom{m}{\mu} \left(\frac{-1}{p}\right)^{\mu} \Phi([\tau^{k+\mu p-1}\,[\tau^{p-1}]^{m-\mu}])\ .
\end{aligned}$$

Since all trees $[\tau^{k+\mu p-1}\,[\tau^{p-1}]^{m-\mu}]$ have $k + mp \leq N$ vertices, we may use the order conditions $\Phi(t) = 1/\gamma(t)$ to obtain

$$\sum_{i=1}^{s} b_i\, c_i^{k-1} \left(A_i^{(p)}\right)^m \;=\; \sum_{\mu=0}^{m} \binom{m}{\mu} \left(\frac{-1}{p}\right)^{\mu} \frac{1}{\gamma([\tau^{k+\mu p-1}\,[\tau^{p-1}]^{m-\mu}])}\ . \tag{2.9}$$

There is a simple argument to show that the combinatorial quantity on the right hand side vanishes for arbitrary $k, m, p \in \mathbb{N}$: consider any Gauss-Legendre method with $s' \geq \max(p, (k + mp)/2)$ stages for which it is well known that $A(s')$ holds. Since $k + mp$ does not exceed order $2s'$, equation (2.9) holds with vanishing left hand side, whence the combination of reciprocal densities on the right hand side vanishes as well.

An analogous argument applies to the equations involving $\tilde{A}_i^{(p)}$. □

For a method of order N with s stages the quantity

$$\nu(N, p) \;=\; \#\,\{(k, m)\ ;\ k, m \in \mathbb{N}\ ,\ k + m\,p \leq N\,\}$$

represents the number of homogeneous equations satisfied by the s components $A_1^{(p)}, \ldots, A_s^{(p)}$ of the simplifying assumption $A(p)$. It is given by

$$\nu(N, p) \;=\; M\left(N - \frac{p\,(M+1)}{2}\right)\ , \quad M \;=\; \lfloor \frac{N-1}{p} \rfloor$$

with $\lfloor\ \rfloor$ denoting the integer part of a real number. If $\nu(N,p) \geq s$, then there are more homogeneous equations than "unknowns" $A_i^{(p)}$. One has to conclude $A_i^{(p)} = 0$, unless the matrix of coefficients $b_i\, c_i^{k-1}$ in these equations is "degenerate". A necessary side condition is the irreducibility assumption $b_i \neq 0$, since the simplifying assumptions only enter via the products $b_i\, A_i^{(p)}$. The values of b_i and c_i are constrained by the quadrature conditions $B(N)$, which often leaves $A_i^{(p)} = 0$ as the only solution of the equations of lemma 2.4. In particular, for self-adjoint methods satisfying (2.4) with the "standard" permutation $\sigma(i) = s+1-i$ this fact can be verified. The self-adjoint methods associated with this permutation are referred to as "standard" in the following theorem.

Theorem 2.5 *For any irreducible standard self-adjoint Runge-Kutta method of order $2n$ with $s \leq 6$ stages the simplifying assumptions $A(p)$ and, equivalently, $\tilde{A}(p)$ hold if $\nu(2n,p) \geq s$.*

Proof We apply a straightforward symbolic computation using the computer algebra system MAPLE V to solve the equations of lemma 2.4 together with the quadrature conditions $\tilde{B}(2n-1)$, which impose constraints on the values of $b_i, \tilde{c}_i$. For given order $2n$, given stage number s and given p with $\nu(2n,p) \geq s$ we consider the system of polynomials

$$\texttt{eqs} := \left\{ \sum_{i=1}^{s} b_i\, \tilde{c}_i^{k-1} - \frac{f_k}{k\, 2^{k-1}} \ ;\ k = 1,\ldots,2n-1 \right\}$$
$$\cup \left\{ \sum_{i=1}^{s} b_i\, \tilde{c}_i^{k-1} \epsilon_i^m \ ;\ k,m \in \mathbb{N}\ ,\ k+mp \leq 2n \right\};$$

In MAPLE this represents a set of equations for the roots of these polynomials involving the unknowns

$$(b_1, b_2, \ldots, b_2, b_1)\ ,\quad (\tilde{c}_1, \tilde{c}_2, \ldots, -\tilde{c}_2, -\tilde{c}_1)\ ,\quad (\epsilon_1, \epsilon_2, \ldots, (-1)^p \epsilon_2, (-1)^p \epsilon_1)\ .$$

The latter represent the simplifying assumptions $\epsilon_i = \tilde{A}_i^{(p)}$, where we note that the symmetry constraints (2.4) imply $\tilde{A}_{\sigma(i)}^{(p)} = (-1)^p \tilde{A}_i^{(p)}$. We use the `gsolve` command in MAPLE's `grobner` package to compute a collection of Gröbner bases:

$$\texttt{solutions} := \texttt{gsolve}(\texttt{eqs}, [b_1, b_2, \ldots, \epsilon_1, \epsilon_2, \ldots, \tilde{c}_1, \tilde{c}_2, \ldots])\ ;$$

MAPLE returns a list of Gröbner bases for different branches of the solution set of `eqs`. We checked that all branches imply $\epsilon_1 = \epsilon_2 = \ldots = 0$ for non-vanishing b_i. This was carried out using MAPLE's `simplify` command using the side relations given by `solutions`:

```
for siderelations in solutions do
   simplify({b1ε1, b2ε2, ...},siderelations);
od;
```

For all cases of n, s, p as given in table 2 the products $b_i \epsilon_i$ are simplified to zero. □

	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$
$s=1$	$A(1)$					
$s=2$	$A(1)$	$A(2)$				
$s=3$	$A(1)$	$A(1)$	$A(3)$			
$s=4$	$A(1)$	$A(1)$	$A(2)$	$A(4)$		
$s=5$	$A(1)$	$A(1)$	$A(2)$	$A(3)$	$A(5)$	
$s=6$	$A(1)$	$A(1)$	$A(2)$	$A(3)$	$A(4)$	$A(6)$

Table 2: Simplifying assumptions implied by order $2n$ with s stages.

We remark that the reason for restricting this computation to self-adjoint methods is to minimize the number of equations and unknowns, since the call of the Gröbner basis routine `gsolve` is doubly exponential in complexity and thus very time consuming. The computation was also carried out for self-adjoint schemes associated with "non-standard" permutations. Following the reasoning of section 4 we tried schemes satisfying (2.4) with representatives of all conjugacy classes in the symmetric group on the indices $\{1,\ldots,s\}$. If was found that theorem 2.5 holds for *all* irreducible self-adjoint methods with $s \leq 6$ stages apart from 3 exceptions related to the conjugacy classes $C_2(5), C_2(6), C_3(6)$. These are discussed in the subsections 4.5.2, 4.6.2 and 4.6.3.

The maximal values of p satisfying $\nu(2n,p) \geq s$ are listed in table 2. One sees that for irreducible standard self-adjoint schemes with $s \leq 6$ stages order $2n$ implies $A(n-1)$ and, equivalently, $\tilde{A}(n-1)$. If these methods are also symplectic, then the sufficient conditions of theorem 2.3 are also *necessary*:

Corollary 2.6 *An irreducible standard symplectic self-adjoint scheme (2.7) with $s \leq 6$ stages is of order $2n$ if and only if $\tilde{B}(2n-1)$ and $\tilde{A}(n-1)$ hold.*

For $s=7$ there exist counter examples of irreducible standard self-adjoint methods of order $2n$ for which $\tilde{A}(n-1)$ does not hold.

3 Classification of standard schemes through 6 stages

A complete list of multi-parameter families of irreducible self-adjoint symplectic Runge-Kutta schemes of standard type (2.7) through 6 stages shall be presented in this section. We briefly sketch the computational procedure used to obtain these results:

0) Starting with the most general standard scheme with arbitrary parameters (b_i), $(\tilde{c}_i)$, (s_{ij}) as given by (2.7) the row-sum conditions $\tilde{A}(1)$ given by (2.3) are implemented: we write

$$s_{ij} \;=\; \tilde{c}_i - \tilde{c}_j \;+\; s_{ij}^{(0)} \;,$$

where $S^{(0)} = (s_{ij}^{(0)})$ is the most general skew-symmetric matrix satisfying the symmetry constraints (2.4) with $\sigma(i) = s+1-i$ and $S^{(0)}\mathbf{b} = 0$. One concludes

$$\tilde{A}(1): \qquad \sum_{j=1}^{s} s_{ij}\, b_j \;=\; \tilde{c}_i \Big(\sum_{j=1}^{s} b_j\Big) \;-\; \sum_{j=1}^{s} b_j\, \tilde{c}_j \;=\; \tilde{c}_i \;, \quad i = 1, \ldots, s$$

assuming the quadrature conditions $\tilde{B}(2)$, i.e., consistency $\sum_j b_j = 1$ together with $\sum_j b_j\, \tilde{c}_j = 0$. We note that the latter is automatically satisfied by virtue of self-adjointness. One regards the condition $S^{(0)}\mathbf{b} = 0$ as a set of homogeneous equations for the components of $S^{(0)}$. Elementary linear algebra leads to the general solution, which is expressed in terms of $\mathbf{b}$ and some free parameters corresponding to the kernel of this linear system.

i) For the classification of the most general family of standard schemes of order $2n$ we first consider the quadrature conditions $\tilde{B}(2n)$ involving the parameters b_i and $\tilde{c}_i$. In fact, according to theorem 2.3 it is sufficient to consider $\tilde{B}(2n-1)$, since all order equations associated with even trees are trivially satisfied due to self-adjointness. Noting that the quadrature conditions are linear in the weights b_i, we use them to express these weights in terms of the abscissae $\tilde{c}_i$. If the order exceeds the stage number, or if some of the $\tilde{c}_i$ coincide, then certain constraints on the parameters $\tilde{c}_i$ arise.

ii) Assume that the most general representation $s_{ij} = s_{ij}(\alpha_1, \alpha_2, \ldots)$ of the Butcher matrix leading to order $2n-2$ was found in a previous step. It involves some arbitrary parameters α_i. Following theorem 2.3 we consider the simplifying assumption $\tilde{A}(n-1)$, which is a system of *linear* equations for the matrix entries s_{ij}, i.e., for the free parameters α_i. Elementary linear algebra leads to the most general solution involving new free parameters $\beta_1, \beta_2, \ldots$ corresponding to the kernel of the linear system. In this step we need to consider the constraints among the weights b_i and the abscissae $\tilde{c}_i$ found in i) in order to determine the rank of the linear system $\tilde{A}(n-1)$. This results in the most general representation $s_{ij} = s_{ij}(\beta_1, \beta_2, \ldots)$ of the Butcher matrix leading to order $2n$ involving a reduced set of free parameters β_i. We note that for $n \le s$ the equations $\tilde{A}(n-1)$ are solvable, since the most general scheme of order $2n$ encompasses the s-stage Gauss-Legendre method which is known to satisfy $\tilde{A}(s)$. Further, since only linear equations have to be solved, the free parameters β_i will enter the general solution $s_{ij} = s_{ij}(\beta_1, \beta_2, \ldots)$ linearly.

iii) A package for automatically generating the order equations was implemented in MAPLE V. The results of the steps i) and ii) were substituted into the order equations. Using MAPLE's `simplify` command with the constraints of step i) as side relations, it was verified that all order equations are indeed satisfied. An independent check was carried out using MATHEMATICA, and equivalent functions which were used are outlined briefly in the appendix.

According to corollary 2.6 this computational procedure leads to *all* standard self-adjoint symplectic schemes with $s \le 6$ stages. The number of free parameters in the main branch of the resulting multi-parameter families of methods is listed in table 3.

	Order					
	2	4	6	8	10	12
$s=1$	0					
$s=2$	1	0				
$s=3$	3	2	0			
$s=4$	5	4	2	0		
$s=5$	8	7	4	2	0	
$s=6$	11	10	7	5	2	0

Table 3: Number of free parameters for the general solution branch of s-stage standard symplectic self-adjoint schemes.

3.1 1 stage

The only consistent symplectic Runge-Kutta scheme with 1 stage is the self-adjoint Gauss-Legendre method of order 2 given by the Butcher tableau

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

It is the classical implicit mid-point rule $\mathbf{y}_n \mapsto \mathbf{y}_{n+1}$ for solving $\frac{d}{dt}\mathbf{y} = \mathbf{f}(t, \mathbf{y})$, where $\mathbf{y}_{n+1}$ is the solution of

$$\mathbf{y}_{n+1} \;=\; \mathbf{y}_n \;+\; h\,\mathbf{f}\Big(\, t_n + \frac{h}{2}\,,\; \frac{1}{2}\,(\mathbf{y}_n + \mathbf{y}_{n+1})\,\Big)\;.$$

3.2 2 stages

The most general form of the 2 stage symplectic standard self-adjoint Butcher tableau is

$$\begin{array}{c|cc} b_1 + \tilde{c}_1 & \frac{b_1}{2} & \frac{b_1}{2} + \tilde{c}_1 \\ b_1 - \tilde{c}_1 & \frac{b_1}{2} - \tilde{c}_1 & \frac{b_1}{2} \\ \hline & b_1 & b_1 \end{array}$$

with order 2 being granted by $b_1 = 1/2$. The only additional constraint $2\,b_1\,\tilde{c}_1^2 = 1/12$ in $\tilde{B}(3)$ leads to the 2 stage Gauss-Legendre method of order 4:

$$\begin{array}{c|cc} \frac{1}{2} \pm \frac{1}{2\sqrt{3}} & \frac{1}{4} & \frac{1}{4} \pm \frac{1}{2\sqrt{3}} \\ \frac{1}{2} \mp \frac{1}{2\sqrt{3}} & \frac{1}{4} \mp \frac{1}{2\sqrt{3}} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

3.3 3 stages

The Butcher tableau for the most general 3 stage symplectic self-adjoint scheme of standard type is

$$\begin{array}{c|ccc} \frac{1}{2} + \tilde{c}_1 & \frac{b_1}{2} & \left(\frac{1}{2} + s_{12}\right) b_2 & \left(\frac{1}{2} + s_{13}\right) b_1 \\ \frac{1}{2} & \left(\frac{1}{2} - s_{12}\right) b_1 & \frac{b_2}{2} & \left(\frac{1}{2} + s_{12}\right) b_1 \\ \frac{1}{2} - \tilde{c}_1 & \left(\frac{1}{2} - s_{13}\right) b_1 & \left(\frac{1}{2} - s_{12}\right) b_2 & \frac{b_1}{2} \\ \hline & b_1 & b_2 & b_1 \end{array} \tag{3.10}$$

with the row-sum conditions (2.3) implemented by

$$s_{12} \;=\; \tilde{c}_1 + \alpha\, b_1\;, \quad s_{13} \;=\; 2\,\tilde{c}_1 - \alpha\, b_2\;. \tag{3.11}$$

It involves 4 free parameters b_1, b_2, $\tilde{c}_1$ and α.

3.3.1 3 stages, order 2

The consistency condition $2\,b_1 + b_2 = 1$ leads to order 2. Elimination of $b_2 = 1 - 2\,b_1$, say, leaves a three-parameter family of methods (3.10)/(3.11).

3.3.2 3 stages, order 4

The only additional constraint $2\,b_1\,\tilde{c}_1^2 = 1/12$ arising from the tree $[\tau^2]$ leads to the family of 4th order schemes (3.10)/(3.11) with

$$b_1 \;=\; \frac{1}{24\,\tilde{c}_1^2}\;, \quad b_2 \;=\; 1 \;-\; \frac{1}{12\,\tilde{c}_1^2}$$

and two arbitrary parameters α and $\tilde{c}_1 \neq 0$.

3.3.3 3 stages, order 6

The conditions $\tilde{B}(5)$ and $\tilde{A}(2)$ fix $\tilde{c}_1^2 = 3/20$ and $\alpha = 9\,\tilde{c}_1/5$. The resulting scheme is the Gauss-Legendre method of order 6:

$$\begin{array}{c|ccc}
\frac{1}{2}+\tilde{c}_1 & \frac{5}{36} & \frac{2}{9}+\frac{2\,\tilde{c}_1}{3} & \frac{5}{36}+\frac{\tilde{c}_1}{3} \\
\frac{1}{2} & \frac{5}{36}-\frac{5\,\tilde{c}_1}{12} & \frac{2}{9} & \frac{5}{36}+\frac{5\,\tilde{c}_1}{12} \\
\frac{1}{2}-\tilde{c}_1 & \frac{5}{36}-\frac{\tilde{c}_1}{3} & \frac{2}{9}-\frac{2\,\tilde{c}_1}{3} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}$$

with $\quad \tilde{c}_1 = \pm\frac{1}{2}\sqrt{\frac{3}{5}}$.

3.4 4 stages

The Butcher tableau for the most general 4 stage symplectic self-adjoint scheme of standard type is

$$\begin{array}{c|cccc}
\frac{1}{2}+\tilde{c}_1 & \frac{b_1}{2} & \left(\frac{1}{2}+s_{12}\right)b_2 & \left(\frac{1}{2}+s_{13}\right)b_2 & \left(\frac{1}{2}+s_{14}\right)b_1 \\
\frac{1}{2}+\tilde{c}_2 & \left(\frac{1}{2}-s_{12}\right)b_1 & \frac{b_2}{2} & \left(\frac{1}{2}+s_{23}\right)b_2 & \left(\frac{1}{2}+s_{13}\right)b_1 \\
\frac{1}{2}-\tilde{c}_2 & \left(\frac{1}{2}-s_{13}\right)b_1 & \left(\frac{1}{2}-s_{23}\right)b_2 & \frac{b_2}{2} & \left(\frac{1}{2}+s_{12}\right)b_1 \\
\frac{1}{2}-\tilde{c}_1 & \left(\frac{1}{2}-s_{14}\right)b_1 & \left(\frac{1}{2}-s_{13}\right)b_2 & \left(\frac{1}{2}-s_{12}\right)b_2 & \frac{b_1}{2} \\
\hline
 & b_1 & b_2 & b_2 & b_1
\end{array} \tag{3.12}$$

with the row-sum conditions (2.3) implemented by

$$\begin{aligned}
s_{12} &= \tilde{c}_1-\tilde{c}_2+\alpha_1\,b_1-\alpha_2\,b_2\ , \quad & s_{14} &= 2\,\tilde{c}_1-2\,\alpha_1\,b_2\ , \\
s_{13} &= \tilde{c}_1+\tilde{c}_2+\alpha_1\,b_1+\alpha_2\,b_2\ , \quad & s_{23} &= 2\,\tilde{c}_2-2\,\alpha_2\,b_1\ .
\end{aligned} \tag{3.13}$$

It involves 6 free parameters b_1, b_2, $\tilde{c}_1$, $\tilde{c}_2$, α_1 and α_2 .

3.4.1 4 stages, order 2

The consistency condition $b_1 + b_2 = 1/2$ arising from the trivial tree τ leads to order 2. Elimination of $b_2 = 1/2 - b_1$, say, leaves a five-parameter family of methods.

3.4.2 4 stages, order 4

The only additional constraint $2\,b_1\,\tilde{c}_1^2 + 2\,b_2\,\tilde{c}_2^2 = 1/12$ arising from the tree $[\tau^2]$ leads to the family of 4th order schemes (3.12)/(3.13) with

$$b_1 \;=\; \frac{1}{24}\,\frac{1-12\,\tilde{c}_2^2}{\tilde{c}_1^2-\tilde{c}_2^2}\,, \quad b_2 \;=\; \frac{1}{24}\,\frac{1-12\,\tilde{c}_1^2}{\tilde{c}_2^2-\tilde{c}_1^2} \tag{3.14}$$

and 4 arbitrary parameters $\alpha_1, \alpha_2, \tilde{c}_1, \tilde{c}_2$, provided $c_1^2 \neq c_2^2$.

A further branch of the solution space is given by

$$b_1 + b_2 \;=\; \frac{1}{2}\,, \quad \tilde{c}_1^2 \;=\; \tilde{c}_2^2 \;=\; \frac{1}{12}\,. \tag{3.15}$$

Elimination of $b_2 = 1/2 - b_1$, say, leaves a three-parameter family of schemes with free parameters α_1, α_2 and b_1.

3.4.3 4 stages, order 6

The quadrature conditions $\tilde{B}(5)$ are not consistent with the assumption $\tilde{c}_1^2 = \tilde{c}_2^2$ underlying (3.15). This only leaves the main branch (3.14) together with the constraint

$$(12\,\tilde{c}_1^2 \,-\, 1)\,(12\,\tilde{c}_2^2 \,-\, 1) \;=\; -\,\frac{4}{5} \tag{3.16}$$

on $\tilde{c}_1$, $\tilde{c}_2$ implying $b_1\,b_2\,(\tilde{c}_1^2 - \tilde{c}_2^2)^2 = 1/720$. A single further equation

$$2\,(\alpha_1\,b_1\,\tilde{c}_1 \;-\; \alpha_2\,b_2\,\tilde{c}_2) \;=\; \tilde{c}_1^2 \;-\; \tilde{c}_2^2$$

arises from the simplifying assumption $\tilde{A}(2)$. It may be resolved by putting

$$\alpha_1 \;=\; 12\,\tilde{c}_1\,(\tilde{c}_1^2-\tilde{c}_2^2) \;+\; \beta\,b_2\,\tilde{c}_2\,, \quad \alpha_2 \;=\; 12\,\tilde{c}_2\,(\tilde{c}_2^2-\tilde{c}_1^2) \;+\; \beta\,b_1\,\tilde{c}_1$$

with an arbitrary parameter β. This defines a two-parameter family of 6th order schemes (3.12) with

$$b_1 \;=\; \frac{1}{24}\,\frac{1-12\,\tilde{c}_2^2}{\tilde{c}_1^2-\tilde{c}_2^2}\,, \quad b_2 \;=\; \frac{1}{24}\,\frac{1-12\,\tilde{c}_1^2}{\tilde{c}_2^2-\tilde{c}_1^2}\,,$$

$$s_{12} \;=\; (\tilde{c}_1-\tilde{c}_2)\left(\frac{3}{2} \;+\; 6\,\tilde{c}_1\,\tilde{c}_2 \;-\; \beta\,b_1\,b_2\right)\,, \quad s_{14} \;=\; 3\,\tilde{c}_1\,(1-4\,\tilde{c}_1^2) \;-\; 2\,\beta\,b_2^2\,\tilde{c}_2\,,$$

$$s_{13} \;=\; (\tilde{c}_1+\tilde{c}_2)\left(\frac{3}{2} \;-\; 6\,\tilde{c}_1\,\tilde{c}_2 \;+\; \beta\,b_1\,b_2\right)\,, \quad s_{23} \;=\; 3\,\tilde{c}_2\,(1-4\,\tilde{c}_2^2) \;-\; 2\,\beta\,b_1^2\,\tilde{c}_1\,.$$

The parameters $\tilde{c}_1$, $\tilde{c}_2$ are subject to the constraint (3.16).

3.4.4 4 stages, order 8

The quadrature conditions $\tilde{B}(7)$ force $\tilde{c}_1, \tilde{c}_2$ to be distinct Legendre roots satisfying

$$560\,\tilde{c}_i^4 - 120\,\tilde{c}_i^2 + 3 \;=\; 0\;, \quad i = 1,2$$

and

$$\tilde{c}_1^2 + \tilde{c}_2^2 \;=\; \frac{3}{14}\;, \quad \tilde{c}_1^2\,\tilde{c}_2^2 \;=\; \frac{3}{560}\;.$$

The simplifying assumption $\tilde{A}(3)$ implies $\beta = -3456\,\tilde{c}_1\tilde{c}_2/49$. The resulting Gauss-Legendre method of order 8 is given by (3.12) with

$$\begin{aligned}
b_1 &= \frac{51 - 140\,\tilde{c}_1^2}{144}\;, \quad s_{12} = (\tilde{c}_1 - \tilde{c}_2)\left(\frac{3}{2} + 10\,\tilde{c}_1\,\tilde{c}_2\right)\;, \quad s_{14} = \frac{\tilde{c}_1}{7}\,(27 - 100\,\tilde{c}_1^2)\;,\\
b_2 &= \frac{51 - 140\,\tilde{c}_2^2}{144}\;, \quad s_{13} = (\tilde{c}_1 + \tilde{c}_2)\left(\frac{3}{2} - 10\,\tilde{c}_1\,\tilde{c}_2\right)\;, \quad s_{23} = \frac{\tilde{c}_2}{7}\,(27 - 100\,\tilde{c}_2^2)\;.
\end{aligned}$$

All parameters are defined up to signs which correspond to a re-ordering of the internal stages. The Legendre roots with $\tilde{c}_1 > \tilde{c}_2 > -\tilde{c}_2 > -\tilde{c}_1$ are given by

$$\tilde{c}_1 \;=\; \sqrt{\frac{3}{28} + \frac{\sqrt{30}}{70}}\;, \quad \tilde{c}_2 \;=\; \sqrt{\frac{3}{28} - \frac{\sqrt{30}}{70}}\;.$$

3.5 5 stages

The Butcher tableau for the most general 5 stage symplectic self-adjoint scheme of standard type is

$$\begin{array}{c|ccccc}
\frac12+\tilde{c}_1 & \frac{b_1}{2} & \left(\frac12+s_{12}\right)b_2 & \left(\frac12+s_{13}\right)b_3 & \left(\frac12+s_{14}\right)b_2 & \left(\frac12+s_{15}\right)b_1\\
\frac12+\tilde{c}_2 & \left(\frac12-s_{12}\right)b_1 & \frac{b_2}{2} & \left(\frac12+s_{23}\right)b_3 & \left(\frac12+s_{24}\right)b_2 & \left(\frac12+s_{14}\right)b_1\\
\frac12 & \left(\frac12-s_{13}\right)b_1 & \left(\frac12-s_{23}\right)b_2 & \frac{b_3}{2} & \left(\frac12+s_{23}\right)b_2 & \left(\frac12+s_{13}\right)b_1\\
\frac12-\tilde{c}_2 & \left(\frac12-s_{14}\right)b_1 & \left(\frac12-s_{24}\right)b_2 & \left(\frac12-s_{23}\right)b_3 & \frac{b_2}{2} & \left(\frac12+s_{12}\right)b_1\\
\frac12-\tilde{c}_1 & \left(\frac12-s_{15}\right)b_1 & \left(\frac12-s_{14}\right)b_2 & \left(\frac12-s_{13}\right)b_3 & \left(\frac12-s_{12}\right)b_2 & \frac{b_1}{2}\\
\hline
 & b_1 & b_2 & b_3 & b_2 & b_1
\end{array} \tag{3.17}$$

with the row-sum conditions (2.3) implemented by

$$\begin{aligned}
s_{12} &= \tilde{c}_1 - \tilde{c}_2 + \sigma_1\,b_1 - \sigma_2\,b_2\;, \quad s_{13} = \tilde{c}_1 + \mu_1\,b_1\;, \quad s_{15} = 2\,\tilde{c}_1 - 2\,\sigma_1\,b_2 - \mu_1\,b_3\;,\\
s_{14} &= \tilde{c}_1 + \tilde{c}_2 + \sigma_1\,b_1 + \sigma_2\,b_2\;, \quad s_{23} = \tilde{c}_2 + \mu_2\,b_2\;, \quad s_{24} = 2\,\tilde{c}_2 - 2\,\sigma_2\,b_1 - \mu_2\,b_3\;.
\end{aligned} \tag{3.18}$$

It involves 9 free parameters $b_1, b_2, b_3,\ \tilde{c}_1, \tilde{c}_2,\ \sigma_1, \sigma_2, \mu_1, \mu_2$.

3.5.1 5 stages, order 2

The consistency condition $2\,b_1 + 2\,b_2 + b_3 = 1$ leads to order 2. Elimination of $b_3 = 1 - 2\,b_1 - 2\,b_2$, say, leaves an eight-parameter family of methods.

3.5.2 5 stages, order 4

The only additional constraint $2\,b_1\,\tilde{c}_1^2 + 2\,b_2\,\tilde{c}_2^2 = 1/12$ arising from the tree $[\tau^2]$ leads to the family of 4th order schemes (3.17)/(3.18) with

$$b_1 \;=\; \frac{1}{24}\,\frac{1 - 12\,(1-b_3)\,c_2^2}{c_1^2 - c_2^2}\;, \qquad b_2 \;=\; \frac{1}{24}\,\frac{1 - 12\,(1-b_3)\,c_1^2}{c_2^2 - c_1^2}$$

and seven free parameters b_3, $\tilde{c}_1, \tilde{c}_2$, σ_1, σ_2, μ_1, μ_2, provided $\tilde{c}_1^2 \neq \tilde{c}_2^2$.

A further branch of the solution set is given by

$$2\,b_1 + 2\,b_2 \;=\; 1 - b_3 \;=\; \frac{1}{12\,\tilde{c}_1^2}\;, \qquad \tilde{c}_2^2 \;=\; \tilde{c}_1^2$$

yielding a family of 4th order schemes with six free parameters.

3.5.3 5 stages, order 6

The quadrature conditions $\tilde{B}(5)$:

$$2\,b_1 + 2\,b_2 + b_3 \;=\; 1\;, \quad 2\,b_1\,\tilde{c}_1^2 + 2\,b_2\,\tilde{c}_2^2 \;=\; \frac{1}{12}\;, \quad 2\,b_1\,\tilde{c}_1^4 + 2\,b_2\,\tilde{c}_2^4 \;=\; \frac{1}{80} \tag{3.19}$$

define b_1, b_2, b_3 in terms of $\tilde{c}_1$, $\tilde{c}_2$ provided $\tilde{c}_1^2$, $\tilde{c}_2^2$ are mutually distinct and non-zero. The simplifying assumption $\tilde{A}(2)$ provides two further equations

$$\begin{aligned} 48\,b_2\,(\,b_1\,\tilde{c}_1\,\sigma_1 \;-\; b_2\,\tilde{c}_2\,\sigma_2\,) \;+\; 24\,b_1\,b_3\,\tilde{c}_1\,\mu_1 \;&=\; 12\,\tilde{c}_1^2 - 1\;, \\ -\,48\,b_1\,(\,b_1\,\tilde{c}_1\,\sigma_1 \;-\; b_2\,\tilde{c}_2\,\sigma_2\,) \;+\; 24\,b_2\,b_3\,\tilde{c}_2\,\mu_2 \;&=\; 12\,\tilde{c}_2^2 - 1\;, \end{aligned} \tag{3.20}$$

which are solved by

$$\begin{aligned} \sigma_1 \;&=\; \frac{\tilde{c}_1 + \alpha_1\,\tilde{c}_2}{2\,b_1}\;, \quad \mu_1 \;=\; \frac{\tilde{c}_1}{2\,b_1} \;-\; \frac{b_2\,\tilde{c}_2}{b_1\,b_3}\,(\alpha_1 - \alpha_2)\;, \\ \sigma_2 \;&=\; \frac{\tilde{c}_2 + \alpha_2\,\tilde{c}_1}{2\,b_2}\;, \quad \mu_2 \;=\; \frac{\tilde{c}_2}{2\,b_2} \;+\; \frac{b_1\,\tilde{c}_1}{b_2\,b_3}\,(\alpha_1 - \alpha_2) \end{aligned}$$

with arbitrary constants α_1, α_2. This leads to the Butcher matrix given by

$$\begin{aligned} s_{12} &= \frac{3}{2}\,(\tilde{c}_1 - \tilde{c}_2) + \frac{\alpha_1\,\tilde{c}_2 - \alpha_2\,\tilde{c}_1}{2}\;, \quad s_{13} = \frac{3}{2}\,\tilde{c}_1 - \frac{b_2\,\tilde{c}_2}{b_3}\,(\alpha_1 - \alpha_2)\;, \\ s_{14} &= \frac{3}{2}\,(\tilde{c}_1 + \tilde{c}_2) + \frac{\alpha_1\,\tilde{c}_2 + \alpha_2\,\tilde{c}_1}{2}\;, \quad s_{23} = \frac{3}{2}\,\tilde{c}_2 + \frac{b_1\,\tilde{c}_1}{b_3}\,(\alpha_1 - \alpha_2)\;, \\ s_{15} &= 3\,\tilde{c}_1 - \frac{\tilde{c}_1}{2\,b_1} - \alpha_2\,\frac{b_2\,\tilde{c}_2}{b_1}\;, \quad s_{24} = 3\,\tilde{c}_2 - \frac{\tilde{c}_2}{2\,b_2} - \alpha_1\,\frac{b_1\,\tilde{c}_1}{b_2}\;. \end{aligned} \tag{3.21}$$

3.5.4 5 stages, order 6, $0 \neq \tilde{c}_1^2 \neq \tilde{c}_2^2 \neq 0$

From (3.19) b_1, b_2, b_3 can be expressed in terms of $\tilde{c}_1$, $\tilde{c}_2$:

$$b_1 \;=\; \frac{1}{480}\,\frac{3-20\,\tilde{c}_2^2}{\tilde{c}_1^2\,(\tilde{c}_1^2-\tilde{c}_2^2)}\;, \quad b_2 \;=\; \frac{1}{480}\,\frac{3-20\,\tilde{c}_1^2}{\tilde{c}_2^2\,(\tilde{c}_2^2-\tilde{c}_1^2)}\;,$$

$$b_3 \;=\; 1-2\,b_1-2\,b_2 \;=\; 1 \;-\; \frac{20\,(\tilde{c}_1^2+\tilde{c}_2^2)-3}{240\,\tilde{c}_1^2\,\tilde{c}_2^2}\;.$$

Together with (3.21) one obtains a family of 6th order schemes (3.17) with four arbitrary parameters $\tilde{c}_1, \tilde{c}_2, \alpha_1, \alpha_2$.

3.5.5 5 stages, order 6, $\tilde{c}_1^2 = \tilde{c}_2^2$

From (3.19) one deduces

$$\tilde{c}_1^2 \;=\; \tilde{c}_2^2 \;=\; \frac{3}{20}\;, \quad b_1+b_2 \;=\; \frac{5}{18}\;, \quad b_3 \;=\; \frac{4}{9}\;.$$

Together with (3.21) one obtains a three-parameter family of 6th order schemes (3.17).

3.5.6 5 stages, order 6, $\tilde{c}_1 = 0$

The equations (3.20) imply $\sigma_2 = \mu_2 = 9\,\tilde{c}_2/5$. In conjunction with (3.19) one obtains a three-parameter family of 6th order schemes (3.17) with

$$\begin{aligned}
&\tilde{c}_1 \;=\; 0\;, \quad \tilde{c}_2^2 \;=\; \frac{3}{20}\;, \quad 2\,b_1+b_3 \;=\; \frac{4}{9}\;, \quad b_2 \;=\; \frac{5}{18}\;,\\
&s_{12} \;=\; -\,\frac{3\,\tilde{c}_2}{2} \;+\; \sigma_1\,b_1\;, \quad s_{23} \;=\; \frac{3\,\tilde{c}_2}{2}\;, \quad s_{13} \;=\; \mu_1\,b_1\;,\\
&s_{14} \;=\; \frac{3\,\tilde{c}_2}{2} \;+\; \sigma_1\,b_1\;, \quad s_{24} \;=\; \frac{6\,\tilde{c}_2}{5}\;, \quad s_{15} \;=\; -\,\frac{5}{9}\,\sigma_1 \;-\; \mu_1\,b_3
\end{aligned}$$

involving the arbitrary constants σ_1, μ_1.

3.5.7 5 stages, order 6, $\tilde{c}_2 = 0$

The equations (3.20) imply $\sigma_1 = \mu_1 = 9\,\tilde{c}_1/5$. In conjunction with (3.19) one obtains the three-parameter family of 6th order schemes (3.17) with

$$\begin{aligned}
&\tilde{c}_2 \;=\; 0\;, \quad \tilde{c}_1^2 \;=\; \frac{3}{20}\;, \quad 2\,b_2+b_3 \;=\; \frac{4}{9}\;, \quad b_1 \;=\; \frac{5}{18}\;,\\
&s_{12} \;=\; \frac{3\,\tilde{c}_1}{2} \;-\; \sigma_2\,b_2\;, \quad s_{13} \;=\; \frac{3\,\tilde{c}_1}{2}\;, \quad s_{23} \;=\; \mu_2\,b_2\;,\\
&s_{14} \;=\; \frac{3\,\tilde{c}_1}{2} \;+\; \sigma_2\,b_2\;, \quad s_{15} \;=\; \frac{6\,\tilde{c}_1}{5}\;, \quad s_{24} \;=\; -\,\frac{5}{9}\,\sigma_2 \;-\; \mu_2\,b_3
\end{aligned}$$

involving the arbitrary constants σ_2, μ_2. These methods are equivalent to those in subsection 3.5.6.

3.5.8 5 stages, order 8

The quadrature conditions $\tilde{B}(7)$ imply that $\tilde{c}_1^2$ and $\tilde{c}_2^2$ are distinct and non-zero. Further, they satisfy the constraint

$$(20\,\tilde{c}_1^2 - 3)\,(20\,\tilde{c}_2^2 - 3) \;=\; -\;\frac{12}{7}\;. \tag{3.22}$$

The simplifying assumption $\tilde{A}(3)$ yields a single equation

$$\alpha_1\,\tilde{c}_2^2 \;-\; \alpha_2\,\tilde{c}_1^2 \;=\; 20\,\tilde{c}_1\,\tilde{c}_2\,(\tilde{c}_1^2 - \tilde{c}_2^2)\;,$$

which is solved by

$$\alpha_1 \;=\; 2\,\beta\,b_3\,\frac{\tilde{c}_1}{\tilde{c}_2} \;-\; 20\,\tilde{c}_1\,\tilde{c}_2\;, \quad \alpha_2 \;=\; 2\,\beta\,b_3\,\frac{\tilde{c}_2}{\tilde{c}_1} \;-\; 20\,\tilde{c}_1\,\tilde{c}_2$$

with an arbitrary parameter β. This yields a two-parameter family of 6th order schemes (3.17) with

$$\begin{aligned}
b_1 \;&=\; \frac{1}{480}\,\frac{3 - 20\,\tilde{c}_2^2}{\tilde{c}_1^2\,(\tilde{c}_1^2 - \tilde{c}_2^2)}\;, \quad b_2 \;=\; \frac{1}{480}\,\frac{3 - 20\,\tilde{c}_1^2}{\tilde{c}_2^2\,(\tilde{c}_2^2 - \tilde{c}_1^2)}\;, \quad b_3 \;=\; \frac{4}{9} \;-\; \frac{1}{420\,\tilde{c}_1^2\,\tilde{c}_2^2}\;,\\
s_{12} \;&=\; (\tilde{c}_1 - \tilde{c}_2)\left(\frac{3}{2} + 10\,\tilde{c}_1\,\tilde{c}_2 + \beta\,b_3\right)\;, \quad s_{13} \;=\; \tilde{c}_1\left(\frac{3}{2} \;-\; 2\,\beta\,b_2\,\frac{\tilde{c}_1^2 - \tilde{c}_2^2}{\tilde{c}_1^2}\right)\;,\\
s_{14} \;&=\; (\tilde{c}_1 + \tilde{c}_2)\left(\frac{3}{2} - 10\,\tilde{c}_1\,\tilde{c}_2 + \beta\,b_3\right)\;, \quad s_{23} \;=\; \tilde{c}_2\left(\frac{3}{2} \;-\; 2\,\beta\,b_1\,\frac{\tilde{c}_2^2 - \tilde{c}_1^2}{\tilde{c}_2^2}\right)\;,\\
s_{15} \;&=\; \frac{\tilde{c}_1}{b_1}\left(\frac{1}{3} + (3 - 20\,\tilde{c}_1^2)\,b_1 - 2\,\beta\,b_2\,b_3\,\frac{\tilde{c}_2^2}{\tilde{c}_1^2}\right)\;,\\
s_{24} \;&=\; \frac{\tilde{c}_2}{b_2}\left(\frac{1}{3} + (3 - 20\,\tilde{c}_2^2)\,b_2 - 2\,\beta\,b_1\,b_3\,\frac{\tilde{c}_1^2}{\tilde{c}_2^2}\right)
\end{aligned}$$

with arbitrary β. The parameters $\tilde{c}_1$, $\tilde{c}_2$ are subject to the constraint (3.22) which may be written as

$$b_1\,b_2\,\tilde{c}_1^2\,\tilde{c}_2^2\,(\tilde{c}_1^2 - \tilde{c}_2^2)^2 \;=\; \frac{1}{134400}$$

implying $b_1 \neq 0$, $b_2 \neq 0$. We note that also those values of $\tilde{c}_1$, $\tilde{c}_2$ leading to $b_3 = 0$ are admissible. These special schemes are equivalent to the 4 stage Gauss-Legendre method.

3.5.9 5 stages, order 10

The quadrature conditions $\tilde{B}(9)$ force $\tilde{c}_1, \tilde{c}_2$ to be distinct Legendre roots satisfying

$$1008\,\tilde{c}_i^4 - 280\,\tilde{c}_i^2 + 15 \;=\; 0\;, \quad i = 1,2$$

and

$$\tilde{c}_1^2 + \tilde{c}_2^2 \;=\; \frac{5}{18}\;, \quad \tilde{c}_1^2\,\tilde{c}_2^2 \;=\; \frac{5}{336}\;.$$

The simplifying assumption $\tilde{A}(4)$ fixes $\beta = 25/16$. The resulting Gauss-Legendre method of order 10 is given by (3.17) with

$$b_1 = \frac{7\,(3+52\,\tilde{c}_2^2)}{400}\;, \quad b_2 = \frac{7\,(3+52\,\tilde{c}_1^2)}{400}\;, \quad b_3 = \frac{64}{225}\;,$$

$$s_{12} = \frac{5\,(\tilde{c}_1-\tilde{c}_2)}{18}\,(7+36\,\tilde{c}_1\,\tilde{c}_2)\;, \quad s_{13} = \frac{5\,\tilde{c}_1}{16}\,(9-28\,\tilde{c}_1^2)\;, \quad s_{15} = \frac{5\,\tilde{c}_1}{81}\,(33-76\,\tilde{c}_1^2)\;,$$

$$s_{14} = \frac{5\,(\tilde{c}_1+\tilde{c}_2)}{18}\,(7-36\,\tilde{c}_1\,\tilde{c}_2)\;, \quad s_{23} = \frac{5\,\tilde{c}_2}{16}\,(9-28\,\tilde{c}_2^2)\;, \quad s_{24} = \frac{5\,\tilde{c}_2}{81}\,(33-76\,\tilde{c}_2^2)\;.$$

All parameters are defined up to signs which correspond to a re-ordering of the internal stages. The Legendre roots with $\tilde{c}_1 > \tilde{c}_2 > -\tilde{c}_2 > -\tilde{c}_1$ are given by

$$\tilde{c}_1 \;=\; \frac{1}{6}\,\sqrt{5 \,+\, \frac{2\,\sqrt{70}}{7}}\;, \quad \tilde{c}_2 \;=\; \frac{1}{6}\,\sqrt{5 \,-\, \frac{2\,\sqrt{70}}{7}}\;.$$

3.6 6 stages

The Butcher tableau for the most general 6 stage symplectic self-adjoint scheme of standard type is

$$\begin{array}{c|cccccc}
\frac12+\tilde{c}_1 & \frac{b_1}{2} & \left(\frac12+s_{12}\right)b_2 & \left(\frac12+s_{13}\right)b_3 & \left(\frac12+s_{14}\right)b_3 & \left(\frac12+s_{15}\right)b_2 & \left(\frac12+s_{16}\right)b_1 \\
\frac12+\tilde{c}_2 & \left(\frac12-s_{12}\right)b_1 & \frac{b_2}{2} & \left(\frac12+s_{23}\right)b_3 & \left(\frac12+s_{24}\right)b_3 & \left(\frac12+s_{25}\right)b_2 & \left(\frac12+s_{15}\right)b_1 \\
\frac12+\tilde{c}_3 & \left(\frac12-s_{13}\right)b_1 & \left(\frac12-s_{23}\right)b_2 & \frac{b_3}{2} & \left(\frac12+s_{34}\right)b_3 & \left(\frac12+s_{24}\right)b_2 & \left(\frac12+s_{14}\right)b_1 \\
\frac12-\tilde{c}_3 & \left(\frac12-s_{14}\right)b_1 & \left(\frac12-s_{24}\right)b_2 & \left(\frac12-s_{34}\right)b_3 & \frac{b_3}{2} & \left(\frac12+s_{23}\right)b_2 & \left(\frac12+s_{13}\right)b_1 \\
\frac12-\tilde{c}_2 & \left(\frac12-s_{15}\right)b_1 & \left(\frac12-s_{25}\right)b_2 & \left(\frac12-s_{24}\right)b_3 & \left(\frac12-s_{23}\right)b_3 & \frac{b_2}{2} & \left(\frac12+s_{12}\right)b_1 \\
\frac12-\tilde{c}_1 & \left(\frac12-s_{16}\right)b_1 & \left(\frac12-s_{15}\right)b_2 & \left(\frac12-s_{14}\right)b_3 & \left(\frac12-s_{13}\right)b_3 & \left(\frac12-s_{12}\right)b_2 & \frac{b_1}{2} \\
\hline
 & b_1 & b_2 & b_3 & b_3 & b_2 & b_1
\end{array}$$

(3.23)

with the row-sum conditions (2.3) implemented by

$$
\begin{aligned}
& s_{12} = \tilde{c}_1 - \tilde{c}_2 + \sigma_1 b_1 - \mu_2 b_2 \ , \quad s_{15} = \tilde{c}_1 + \tilde{c}_2 + \sigma_1 b_1 + \mu_2 b_2 \ , \\
& s_{13} = \tilde{c}_1 - \tilde{c}_3 - \sigma_3 b_3 + \mu_1 b_1 \ , \quad s_{14} = \tilde{c}_1 + \tilde{c}_3 + \sigma_3 b_3 + \mu_1 b_1 \ , \\
& s_{23} = \tilde{c}_2 - \tilde{c}_3 + \sigma_2 b_2 - \mu_3 b_3 \ , \quad s_{24} = \tilde{c}_2 + \tilde{c}_3 + \sigma_2 b_2 + \mu_3 b_3 \ , \\
& \qquad s_{16} = 2\,\tilde{c}_1 - 2\,\sigma_1 b_2 - 2\,\mu_1 b_3 \ , \\
& \qquad s_{25} = 2\,\tilde{c}_2 - 2\,\sigma_2 b_3 - 2\,\mu_2 b_1 \ , \\
& \qquad s_{34} = 2\,\tilde{c}_3 - 2\,\sigma_3 b_1 - 2\,\mu_3 b_2 \ .
\end{aligned}
\tag{3.24}
$$

It involves 12 free parameters b_1, b_2, b_3, $\tilde{c}_1$, $\tilde{c}_2$, $\tilde{c}_3$, σ_1, σ_2, σ_3, μ_1, μ_2, μ_3.

3.6.1 6 stages, order 2

The consistency condition $b_1 + b_2 + b_3 = 1/2$ leads to order 2. Elimination of $b_3 = 1/2 - b_1 - b_2$, say, leaves an eleven-parameter family of methods.

For higher orders the general solution of the order equations branches into several cases, depending on whether some of the values $\tilde{c}_1^2$, $\tilde{c}_2^2$, $\tilde{c}_3^2$ coincide. We first consider the main branch in which these values are mutually distinct.

3.6.2 6 stages, order 4, $\tilde{c}_1^2$, $\tilde{c}_2^2$, $\tilde{c}_3^2$ mutually distinct

The quadrature conditions $\tilde{B}(5)$ lead lead to a family of 4th order schemes (3.23)/(3.24) with

$$
b_1 \ = \ \frac{1 - 12\,\tilde{c}_2^2 + 24\,b_3\,(\tilde{c}_2^2 - \tilde{c}_3^2)}{24\,(\tilde{c}_1^2 - \tilde{c}_2^2)} \ , \quad b_2 \ = \ \frac{1 - 12\,\tilde{c}_1^2 + 24\,b_3\,(\tilde{c}_1^2 - \tilde{c}_3^2)}{24\,(\tilde{c}_2^2 - \tilde{c}_1^2)}
$$

and 10 arbitrary parameters $\sigma_1, \sigma_2, \sigma_3$, μ_1, μ_2, μ_3, b_3 and $\tilde{c}_1$, $\tilde{c}_2$, $\tilde{c}_3$.

3.6.3 6 stages, order 6, $\tilde{c}_1^2$, $\tilde{c}_2^2$, $\tilde{c}_3^2$ mutually distinct

The simplifying assumption $\tilde{A}(2)$ has rank 2 and is solved by replacing the six parameters $\sigma_1, \sigma_2, \sigma_3$, μ_1, μ_2, μ_3 by four arbitrary parameters $\alpha_0, \alpha_1, \alpha_2, \alpha_3$:

$$
\begin{aligned}
\sigma_1 &= \frac{1}{b_1}\left(\frac{1}{2}\,\tilde{c}_1 + \alpha_3\,\tilde{c}_2 + \alpha_0\,b_3\,\tilde{c}_2\,\tilde{c}_3\right) \ , \quad \mu_1 = \frac{1}{b_1}\left(\frac{1}{2}\,\tilde{c}_1 + \alpha_2\,\tilde{c}_3 - \alpha_0\,b_2\,\tilde{c}_2\,\tilde{c}_3\right) \ , \\
\sigma_2 &= \frac{1}{b_2}\left(\frac{1}{2}\,\tilde{c}_2 + \alpha_1\,\tilde{c}_3 + \alpha_0\,b_1\,\tilde{c}_1\,\tilde{c}_3\right) \ , \quad \mu_2 = \frac{1}{b_2}\left(\frac{1}{2}\,\tilde{c}_2 + \alpha_3\,\tilde{c}_1 - \alpha_0\,b_3\,\tilde{c}_1\,\tilde{c}_3\right) \ , \\
\sigma_3 &= \frac{1}{b_3}\left(\frac{1}{2}\,\tilde{c}_3 + \alpha_2\,\tilde{c}_1 + \alpha_0\,b_2\,\tilde{c}_1\,\tilde{c}_2\right) \ , \quad \mu_3 = \frac{1}{b_3}\left(\frac{1}{2}\,\tilde{c}_3 + \alpha_1\,\tilde{c}_2 - \alpha_0\,b_1\,\tilde{c}_1\,\tilde{c}_2\right) \ .
\end{aligned}
$$

The quadrature conditions $\tilde{B}(5)$ yield

$$b_1 \;=\; \frac{3-20\,\tilde c_2^2-20\,\tilde c_3^2+240\,\tilde c_2^2\tilde c_3^2}{480\,(\tilde c_1^2-\tilde c_2^2)\,(\tilde c_1^2-\tilde c_3^2)}\;,\quad b_2 \;=\; \frac{3-20\,\tilde c_1^2-20\,\tilde c_3^2+240\,\tilde c_1^2\tilde c_3^2}{480\,(\tilde c_2^2-\tilde c_1^2)\,(\tilde c_2^2-\tilde c_3^2)}\;,$$

$$b_3 \;=\; \frac{3-20\,\tilde c_1^2-20\,\tilde c_2^2+240\,\tilde c_1^2\tilde c_2^2}{480\,(\tilde c_3^2-\tilde c_1^2)\,(\tilde c_3^2-\tilde c_2^2)}\;.$$

Together with

$$\begin{aligned}
s_{12} &= (\tilde c_1-\tilde c_2)\left(\frac{3}{2}\;-\;\alpha_3\right)\;+\;\alpha_0\,b_3\,\tilde c_3\,(\tilde c_1+\tilde c_2)\;,\\
s_{13} &= (\tilde c_1-\tilde c_3)\left(\frac{3}{2}\;-\;\alpha_2\right)\;-\;\alpha_0\,b_2\,\tilde c_2\,(\tilde c_1+\tilde c_3)\;,\\
s_{14} &= (\tilde c_1+\tilde c_3)\left(\frac{3}{2}\;+\;\alpha_2\right)\;+\;\alpha_0\,b_2\,\tilde c_2\,(\tilde c_1-\tilde c_3)\;,\\
s_{15} &= (\tilde c_1+\tilde c_2)\left(\frac{3}{2}\;+\;\alpha_3\right)\;-\;\alpha_0\,b_3\,\tilde c_3\,(\tilde c_1-\tilde c_2)\;,\\
s_{23} &= (\tilde c_2-\tilde c_3)\left(\frac{3}{2}\;-\;\alpha_1\right)\;+\;\alpha_0\,b_1\,\tilde c_1\,(\tilde c_2+\tilde c_3)\;,\\
s_{24} &= (\tilde c_2+\tilde c_3)\left(\frac{3}{2}\;+\;\alpha_1\right)\;-\;\alpha_0\,b_1\,\tilde c_1\,(\tilde c_2-\tilde c_3)\;,\\
s_{16} &= 3\,\tilde c_1\;-\;\frac{1}{2\,b_1}\,(\tilde c_1+4\,\alpha_2\,b_3\,\tilde c_3+4\,\alpha_3\,b_2\,\tilde c_2)\;,\\
s_{25} &= 3\,\tilde c_2\;-\;\frac{1}{2\,b_2}\,(\tilde c_2+4\,\alpha_3\,b_1\,\tilde c_1+4\,\alpha_1\,b_3\,\tilde c_3)\;,\\
s_{34} &= 3\,\tilde c_3\;-\;\frac{1}{2\,b_3}\,(\tilde c_3+4\,\alpha_1\,b_2\,\tilde c_2+4\,\alpha_2\,b_1\,\tilde c_1)
\end{aligned}\tag{3.25}$$

one obtains a family of 6th order methods (3.23) with seven arbitrary parameters $\tilde c_1, \tilde c_2, \tilde c_3$, $\alpha_0, \alpha_1, \alpha_2, \alpha_3$.

3.6.4 6 stages, order 8, $\tilde c_1^2$, $\tilde c_2^2$, $\tilde c_3^2$ mutually distinct

The simplifying assumption $\tilde{A}(3)$ has rank 2 and is solved by putting

$$\begin{aligned}
\alpha_0 &= \frac{\gamma}{2}\,(\tilde c_1^2-\tilde c_2^2)\,(\tilde c_2^2-\tilde c_3^2)\,(\tilde c_3^2-\tilde c_1^2)\;,\\
\alpha_1 &= \left(\beta-\;\frac{\gamma}{2}\,(\tilde c_2^2+\tilde c_3^2)\right)\,b_1\,\tilde c_1\,(\tilde c_1^2-\tilde c_2^2)\,(\tilde c_1^2-\tilde c_3^2)\;-\;10\,\tilde c_2\,\tilde c_3\;,\\
\alpha_2 &= \left(\beta-\;\frac{\gamma}{2}\,(\tilde c_1^2+\tilde c_3^2)\right)\,b_2\,\tilde c_2\,(\tilde c_2^2-\tilde c_1^2)\,(\tilde c_2^2-\tilde c_3^2)\;-\;10\,\tilde c_1\,\tilde c_3\;,\\
\alpha_3 &= \left(\beta-\;\frac{\gamma}{2}\,(\tilde c_1^2+\tilde c_2^2)\right)\,b_3\,\tilde c_3\,(\tilde c_3^2-\tilde c_1^2)\,(\tilde c_3^2-\tilde c_2^2)\;-\;10\,\tilde c_1\,\tilde c_2
\end{aligned}$$

with arbitrary parameters β, γ. One finds a four-parameter family of 8th order methods (3.23) with

$$
\begin{aligned}
b_1 &= \frac{3 - 20\,\tilde c_2^2 - 20\,\tilde c_3^2 + 240\,\tilde c_2^2 \tilde c_3^2}{480\,(\tilde c_1^2 - \tilde c_2^2)\,(\tilde c_1^2 - \tilde c_3^2)}\,, \quad b_2 = \frac{3 - 20\,\tilde c_1^2 - 20\,\tilde c_3^2 + 240\,\tilde c_1^2 \tilde c_3^2}{480\,(\tilde c_2^2 - \tilde c_1^2)\,(\tilde c_2^2 - \tilde c_3^2)}\,, \\
b_3 &= \frac{3 - 20\,\tilde c_1^2 - 20\,\tilde c_2^2 + 240\,\tilde c_1^2 \tilde c_2^2}{480\,(\tilde c_3^2 - \tilde c_1^2)\,(\tilde c_3^2 - \tilde c_2^2)}\,, \\
s_{12} &= (\tilde c_1 - \tilde c_2)\left(\frac{3}{2} + 10\,\tilde c_1\,\tilde c_2 + (\gamma\,\tilde c_1\,\tilde c_2 + \beta)\,b_3\,\tilde c_3\,(\tilde c_1^2 - \tilde c_3^2)\,(\tilde c_3^2 - \tilde c_2^2)\right)\,, \\
s_{13} &= (\tilde c_1 - \tilde c_3)\left(\frac{3}{2} + 10\,\tilde c_1\,\tilde c_3 + (\gamma\,\tilde c_1\,\tilde c_3 + \beta)\,b_2\,\tilde c_2\,(\tilde c_1^2 - \tilde c_2^2)\,(\tilde c_2^2 - \tilde c_3^2)\right)\,, \\
s_{14} &= (\tilde c_1 + \tilde c_3)\left(\frac{3}{2} - 10\,\tilde c_1\,\tilde c_3 + (\gamma\,\tilde c_1\,\tilde c_3 - \beta)\,b_2\,\tilde c_2\,(\tilde c_1^2 - \tilde c_2^2)\,(\tilde c_2^2 - \tilde c_3^2)\right)\,, \\
s_{15} &= (\tilde c_1 + \tilde c_2)\left(\frac{3}{2} - 10\,\tilde c_1\,\tilde c_2 + (\gamma\,\tilde c_1\,\tilde c_2 - \beta)\,b_3\,\tilde c_3\,(\tilde c_1^2 - \tilde c_3^2)\,(\tilde c_3^2 - \tilde c_2^2)\right)\,, \\
s_{23} &= (\tilde c_2 - \tilde c_3)\left(\frac{3}{2} + 10\,\tilde c_2\,\tilde c_3 + (\gamma\,\tilde c_2\,\tilde c_3 + \beta)\,b_1\,\tilde c_1\,(\tilde c_3^2 - \tilde c_1^2)\,(\tilde c_1^2 - \tilde c_2^2)\right)\,, \\
s_{24} &= (\tilde c_2 + \tilde c_3)\left(\frac{3}{2} - 10\,\tilde c_2\,\tilde c_3 + (\gamma\,\tilde c_2\,\tilde c_3 - \beta)\,b_1\,\tilde c_1\,(\tilde c_2^2 - \tilde c_1^2)\,(\tilde c_1^2 - \tilde c_3^2)\right)\,, \\
s_{16} &= 3\,\tilde c_1 - 20\,\tilde c_1^3 + \frac{\tilde c_1}{3\,b_1} + (\gamma\,\tilde c_1^2 - \beta)\,\frac{2\,b_2\,b_3}{b_1}\,\tilde c_2\,\tilde c_3\,(\tilde c_2^2 - \tilde c_3^2)^2\,, \\
s_{25} &= 3\,\tilde c_2 - 20\,\tilde c_2^3 + \frac{\tilde c_2}{3\,b_2} + (\gamma\,\tilde c_2^2 - \beta)\,\frac{2\,b_1\,b_3}{b_2}\,\tilde c_1\,\tilde c_3\,(\tilde c_1^2 - \tilde c_3^2)^2\,, \\
s_{34} &= 3\,\tilde c_3 - 20\,\tilde c_3^3 + \frac{\tilde c_3}{3\,b_3} + (\gamma\,\tilde c_3^2 - \beta)\,\frac{2\,b_1\,b_2}{b_3}\,\tilde c_1\,\tilde c_2\,(\tilde c_1^2 - \tilde c_2^2)^2\,,
\end{aligned}
$$

where β and γ are arbitrary and $\tilde c_1$, $\tilde c_2$, $\tilde c_3$ are subject to the constraint

$$
3\,(\tilde c_1^2 + \tilde c_2^2 + \tilde c_3^2) \;-\; 20\,(\tilde c_2^2\,\tilde c_3^2 + \tilde c_1^2\,\tilde c_3^2 + \tilde c_1^2\,\tilde c_2^2) \;+\; 240\,\tilde c_1^2\,\tilde c_2^2\,\tilde c_3^2 \;=\; \frac{15}{28}
$$

induced by $\tilde B(7)$.

3.6.5 6 stages, order 10

The quadrature conditions $\tilde B(9)$ imply

$$
b_1\,b_2\,b_3\,(\tilde c_1^2 - \tilde c_2^2)^2\,(\tilde c_2^2 - \tilde c_3^2)^2\,(\tilde c_3^2 - \tilde c_1^2)^2 \;=\; \frac{1}{63\,504\,000}\,,
$$

whence the values $\tilde c_1^2$, $\tilde c_2^2$, $\tilde c_3^2$ are necessarily distinct. The simplifying assumption $\tilde A(4)$ has rank 1 and leads to the single constraint $\gamma\,\tilde c_1 \tilde c_2 \tilde c_3 = -210$. One obtains a two-parameter family of methods (3.23) with

$$
b_1 = \frac{3 - 20\,\tilde c_2^2 - 20\,\tilde c_3^2 + 240\,\tilde c_2^2 \tilde c_3^2}{480\,(\tilde c_1^2 - \tilde c_2^2)\,(\tilde c_1^2 - \tilde c_3^2)}\,, \quad b_2 = \frac{3 - 20\,\tilde c_1^2 - 20\,\tilde c_3^2 + 240\,\tilde c_1^2 \tilde c_3^2}{480\,(\tilde c_2^2 - \tilde c_1^2)\,(\tilde c_2^2 - \tilde c_3^2)}\,,
$$

$$
\begin{aligned}
b_3 &= \frac{3 - 20\,\tilde c_1^2 - 20\,\tilde c_2^2 + 240\,\tilde c_1^2 \tilde c_2^2}{480\,(\tilde c_3^2 - \tilde c_1^2)\,(\tilde c_3^2 - \tilde c_2^2)}\;,\\
s_{12} &= (\tilde c_1 - \tilde c_2)\,\left(\frac{3}{2} + 10\,\tilde c_1\,\tilde c_2 + (\beta\,\tilde c_3 - 210)\,b_3\,(\tilde c_1^2 - \tilde c_3^2)\,(\tilde c_3^2 - \tilde c_2^2)\right)\;,\\
s_{13} &= (\tilde c_1 - \tilde c_3)\,\left(\frac{3}{2} + 10\,\tilde c_1\,\tilde c_3 + (\beta\,\tilde c_2 - 210)\,b_2\,(\tilde c_1^2 - \tilde c_2^2)\,(\tilde c_2^2 - \tilde c_3^2)\right)\;,\\
s_{14} &= (\tilde c_1 + \tilde c_3)\,\left(\frac{3}{2} - 10\,\tilde c_1\,\tilde c_3 - (\beta\,\tilde c_2 + 210)\,b_2\,(\tilde c_1^2 - \tilde c_2^2)\,(\tilde c_2^2 - \tilde c_3^2)\right)\;,\\
s_{15} &= (\tilde c_1 + \tilde c_2)\,\left(\frac{3}{2} - 10\,\tilde c_1\,\tilde c_2 - (\beta\,\tilde c_3 + 210)\,b_3\,(\tilde c_1^2 - \tilde c_3^2)\,(\tilde c_3^2 - \tilde c_2^2)\right)\;,\\
s_{23} &= (\tilde c_2 - \tilde c_3)\,\left(\frac{3}{2} + 10\,\tilde c_2\,\tilde c_3 + (\beta\,\tilde c_1 - 210)\,b_1\,(\tilde c_3^2 - \tilde c_1^2)\,(\tilde c_1^2 - \tilde c_2^2)\right)\;,\\
s_{24} &= (\tilde c_2 + \tilde c_3)\,\left(\frac{3}{2} - 10\,\tilde c_2\,\tilde c_3 - (\beta\,\tilde c_1 + 210)\,b_1\,(\tilde c_2^2 - \tilde c_1^2)\,(\tilde c_1^2 - \tilde c_3^2)\right)\;,\\
s_{16} &= 3\,\tilde c_1 \;-\; 20\,\tilde c_1^3 \;+\; \frac{\tilde c_1}{3\,b_1} \;-\; (\beta\,\tilde c_2\,\tilde c_3 + 210\,\tilde c_1)\,\frac{2\,b_2\,b_3}{b_1}\,(\tilde c_2^2 - \tilde c_3^2)^2\;,\\
s_{25} &= 3\,\tilde c_2 \;-\; 20\,\tilde c_2^3 \;+\; \frac{\tilde c_2}{3\,b_2} \;-\; (\beta\,\tilde c_1\,\tilde c_3 + 210\,\tilde c_2)\,\frac{2\,b_1\,b_3}{b_2}\,(\tilde c_1^2 - \tilde c_3^2)^2\;,\\
s_{34} &= 3\,\tilde c_3 \;-\; 20\,\tilde c_3^3 \;+\; \frac{\tilde c_3}{3\,b_3} \;-\; (\beta\,\tilde c_1\,\tilde c_2 + 210\,\tilde c_3)\,\frac{2\,b_1\,b_2}{b_3}\,(\tilde c_1^2 - \tilde c_2^2)^2\;,
\end{aligned}
$$

where β is arbitrary and $\tilde c_1$, $\tilde c_2$, $\tilde c_3$ are subject to the constraints

$$
\begin{aligned}
&3\,(\tilde c_1^2 + \tilde c_2^2 + \tilde c_3^2) \;-\; 20\,(\tilde c_2^2\,\tilde c_3^2 + \tilde c_1^2\,\tilde c_3^2 + \tilde c_1^2\,\tilde c_2^2) \;+\; 240\,\tilde c_1^2\,\tilde c_2^2\,\tilde c_3^2 \;=\; \frac{15}{28}\;,\\
&3\,(\tilde c_1^2 + \tilde c_2^2 + \tilde c_3^2) \;-\; 14\,(\tilde c_2^2\,\tilde c_3^2 + \tilde c_1^2\,\tilde c_3^2 + \tilde c_1^2\,\tilde c_2^2) \;=\; \frac{5}{8}
\end{aligned}
$$

implied by $\tilde B(9)$.

3.6.6 6 stages, order 12

The quadrature conditions $\tilde B(11)$ lead to

$$
b_i = \frac{23}{96} - \frac{28\,\tilde c_i^2}{75} - \frac{77\,\tilde c_i^4}{50}\;, \quad i = 1, 2, 3\;,
$$

with the distinct Legendre roots $\tilde c_i$ satisfying

$$
14\,784\;\tilde c_i^6 \;-\; 5\,040\;\tilde c_i^4 \;+\; 420\;\tilde c_i^2 \;=\; 5\;, \quad i = 1, 2, 3
$$

and

$$
\tilde c_1^2 + \tilde c_2^2 + \tilde c_3^2 \;=\; \frac{15}{44}\;, \quad \tilde c_1^2\,\tilde c_2^2\,\tilde c_3^2 \;=\; \frac{5}{14\,784}\;.
$$

The simplifying assumption $\tilde{A}(5)$ leads to $\beta\,\tilde{c}_1\tilde{c}_2\tilde{c}_3 = -225/22$. One obtains the Gauss-Legendre method (3.23) with

$$s_{12} = \frac{\tilde{c}_1 - \tilde{c}_2}{16}\Big(45 - 140\,(\tilde{c}_1^2 - 5\,\tilde{c}_1\tilde{c}_2 + \tilde{c}_2^2) + 336\,\tilde{c}_1\tilde{c}_2\,(\,60\,\tilde{c}_1^2\tilde{c}_2^2 + 5\,\tilde{c}_1\tilde{c}_2 - 9\,\tilde{c}_1^2 - 9\,\tilde{c}_2^2\,)\Big)\,,$$
$$s_{13} = \frac{\tilde{c}_1 - \tilde{c}_3}{16}\Big(45 - 140\,(\tilde{c}_1^2 - 5\,\tilde{c}_1\tilde{c}_3 + \tilde{c}_3^2) + 336\,\tilde{c}_1\tilde{c}_3\,(\,60\,\tilde{c}_1^2\tilde{c}_3^2 + 5\,\tilde{c}_1\tilde{c}_3 - 9\,\tilde{c}_1^2 - 9\,\tilde{c}_3^2\,)\Big)\,,$$
$$s_{14} = \frac{\tilde{c}_1 + \tilde{c}_3}{16}\Big(45 - 140\,(\tilde{c}_1^2 + 5\,\tilde{c}_1\tilde{c}_3 + \tilde{c}_3^2) - 336\,\tilde{c}_1\tilde{c}_3\,(\,60\,\tilde{c}_1^2\tilde{c}_3^2 - 5\,\tilde{c}_1\tilde{c}_3 - 9\,\tilde{c}_1^2 - 9\,\tilde{c}_3^2\,)\Big)\,,$$
$$s_{15} = \frac{\tilde{c}_1 + \tilde{c}_2}{16}\Big(45 - 140\,(\tilde{c}_1^2 + 5\,\tilde{c}_1\tilde{c}_2 + \tilde{c}_2^2) - 336\,\tilde{c}_1\tilde{c}_2\,(\,60\,\tilde{c}_1^2\tilde{c}_2^2 - 5\,\tilde{c}_1\tilde{c}_2 - 9\,\tilde{c}_1^2 - 9\,\tilde{c}_2^2\,)\Big)\,,$$
$$s_{23} = \frac{\tilde{c}_2 - \tilde{c}_3}{16}\Big(45 - 140\,(\tilde{c}_2^2 - 5\,\tilde{c}_2\tilde{c}_3 + \tilde{c}_3^2) + 336\,\tilde{c}_2\tilde{c}_3\,(\,60\,\tilde{c}_2^2\tilde{c}_3^2 + 5\,\tilde{c}_2\tilde{c}_3 - 9\,\tilde{c}_2^2 - 9\,\tilde{c}_3^2\,)\Big)\,,$$
$$s_{24} = \frac{\tilde{c}_2 + \tilde{c}_3}{16}\Big(45 - 140\,(\tilde{c}_2^2 + 5\,\tilde{c}_2\tilde{c}_3 + \tilde{c}_3^2) - 336\,\tilde{c}_2\tilde{c}_3\,(\,60\,\tilde{c}_2^2\tilde{c}_3^2 - 5\,\tilde{c}_2\tilde{c}_3 - 9\,\tilde{c}_2^2 - 9\,\tilde{c}_3^2\,)\Big)\,,$$
$$s_{16} = \frac{\tilde{c}_1}{968}\,(5475 - 51\,800\;\tilde{c}_1^2 + 144\,816\;\tilde{c}_1^4)\,,$$
$$s_{25} = \frac{\tilde{c}_2}{968}\,(5475 - 51\,800\;\tilde{c}_2^2 + 144\,816\;\tilde{c}_2^4)\,,$$
$$s_{34} = \frac{\tilde{c}_3}{968}\,(5475 - 51\,800\;\tilde{c}_3^2 + 144\,816\;\tilde{c}_3^4)\,.$$

3.6.7 6 stages, $\tilde{c}_1^2 \neq \tilde{c}_2^2 = \tilde{c}_3^2$

We now consider subbranches of the solution space corresponding to coinciding values of $\tilde{c}_1^2$, $\tilde{c}_2^2$, $\tilde{c}_3^2$. First, we assume that two of these values coincide and are not equal to the third. We may assume $\tilde{c}_1^2 \neq \tilde{c}_2^2 = \tilde{c}_3^2$, since all other cases lead to the same Runge-Kutta scheme after an appropriate permutation of the indices 1,2,3.

Order 4: One finds the methods of subsection 3.6.2 with 9 arbitrary parameters $\sigma_1, \sigma_2, \sigma_3$, μ_1, μ_2, μ_3, b_3 and $\tilde{c}_1$, $\tilde{c}_2$.

Order 6: The quadrature conditions $\tilde{B}(5)$ lead to

$$b_1 \;=\; \frac{1}{24}\,\frac{1 - 12\,\tilde{c}_2^2}{\tilde{c}_1^2 - \tilde{c}_2^2}\,,\quad b_2 \;=\; \frac{1}{48}\,\frac{1 - 12\,\tilde{c}_1^2 + b}{\tilde{c}_2^2 - \tilde{c}_1^2}\,,\quad b_3 \;=\; \frac{1}{48}\,\frac{1 - 12\,\tilde{c}_1^2 - b}{\tilde{c}_2^2 - \tilde{c}_1^2}$$

with an arbitrary parameter b and the constraints

$$\tilde{c}_3^2 \;=\; \tilde{c}_2^2\,,\quad \tilde{c}_1^2 \;+\; \tilde{c}_2^2 \;-\; 12\,\tilde{c}_1^2\,\tilde{c}_2^2 \;=\; \frac{3}{20}\,.$$

This leaves one degree of freedom in the parameters $\tilde{c}_1$, $\tilde{c}_2$, $\tilde{c}_3$. Together with (3.25) one obtains a six parameter family of 6th order methods (3.23) with arbitrary constants b,

$\alpha_0, \alpha_1, \alpha_2, \alpha_3$.

Order 8: The quadrature conditions $\tilde{B}(7)$ lead to the constraints

$$\tilde{c}_3^2 = \tilde{c}_2^2 , \quad \tilde{c}_1^2 \tilde{c}_2^2 = \frac{3}{560} , \quad \tilde{c}_1^2 + \tilde{c}_2^2 = \frac{3}{14} ,$$

i.e.,

$$\tilde{c}_1^2 = \frac{3}{28} \pm \frac{\sqrt{30}}{70} , \quad \tilde{c}_2^2 = \tilde{c}_3^2 = \frac{3}{28} \mp \frac{\sqrt{30}}{70} .$$

For (3.25) the simplifying assumption $\tilde{A}(3)$ has rank 2 and is solved by putting

$$\alpha_1 = -10\, \tilde{c}_2\, \tilde{c}_3 + \delta , \quad \alpha_2 = -10\, \tilde{c}_1\, \tilde{c}_3 - \alpha_0\, b_2\, \tilde{c}_2 , \quad \alpha_3 = -10\, \tilde{c}_1\, \tilde{c}_2 + \alpha_0\, b_3\, \tilde{c}_3 .$$

With

$$b_1 = \frac{1}{24}\, \frac{1 - 12\, \tilde{c}_2^2}{\tilde{c}_1^2 - \tilde{c}_2^2} , \quad b_2 = \frac{1}{48}\, \frac{1 - 12\, \tilde{c}_1^2 + b}{\tilde{c}_2^2 - \tilde{c}_1^2} , \quad b_3 = \frac{1}{48}\, \frac{1 - 12\, \tilde{c}_1^2 - b}{\tilde{c}_2^2 - \tilde{c}_1^2} ,$$

$$\begin{aligned}
s_{12} &= (\tilde{c}_1 - \tilde{c}_2) \left(\frac{3}{2} + 10\, \tilde{c}_1\, \tilde{c}_2 \right) + 2\, \alpha_0\, b_3\, \tilde{c}_2\, \tilde{c}_3 , \\
s_{13} &= (\tilde{c}_1 - \tilde{c}_3) \left(\frac{3}{2} + 10\, \tilde{c}_1\, \tilde{c}_3 \right) - 2\, \alpha_0\, b_2\, \tilde{c}_2\, \tilde{c}_3 , \\
s_{14} &= (\tilde{c}_1 + \tilde{c}_3) \left(\frac{3}{2} - 10\, \tilde{c}_1\, \tilde{c}_3 \right) - 2\, \alpha_0\, b_2\, \tilde{c}_2\, \tilde{c}_3 , \\
s_{15} &= (\tilde{c}_1 + \tilde{c}_2) \left(\frac{3}{2} - 10\, \tilde{c}_1\, \tilde{c}_2 \right) + 2\, \alpha_0\, b_3\, \tilde{c}_2\, \tilde{c}_3 , \\
s_{23} &= (\tilde{c}_2 - \tilde{c}_3) \left(\frac{3}{2} + 10\, \tilde{c}_2\, \tilde{c}_3 - \delta \right) + \alpha_0\, b_1\, \tilde{c}_1\, (\tilde{c}_2 + \tilde{c}_3) , \\
s_{24} &= (\tilde{c}_2 + \tilde{c}_3) \left(\frac{3}{2} - 10\, \tilde{c}_2\, \tilde{c}_3 + \delta \right) - \alpha_0\, b_1\, \tilde{c}_1\, (\tilde{c}_2 - \tilde{c}_3) , \\
s_{16} &= \tilde{c}_1 \left(3 - 20\, \tilde{c}_1^2 + \frac{1}{3\, b_1} \right) , \\
s_{25} &= \tilde{c}_2 \left(3 - 20\, \tilde{c}_2^2 + \frac{1}{3\, b_2} \right) - \frac{2\, b_3\, \tilde{c}_3}{b_2} (\delta + \alpha_0\, b_1\, \tilde{c}_1) , \\
s_{34} &= \tilde{c}_3 \left(3 - 20\, \tilde{c}_3^2 + \frac{1}{3\, b_3} \right) - \frac{2\, b_2\, \tilde{c}_2}{b_3} (\delta - \alpha_0\, b_1\, \tilde{c}_1)
\end{aligned}$$

one obtains a three-parameter family of 8th order schemes (3.23) with arbitrary b, α_0 and δ. We note that the abscissae $\tilde{c}_i$ coincide with those of the 4 stage Gauss-Legendre method of subsection 3.4.4. For $b = \pm(12\, \tilde{c}_1^2 - 1)$, i.e., either $b_2 = 0$ or $b_3 = 0$, the second, respectively third, of the internal stages $\mathbf{y^{(i)}}$ in (2.1) becomes redundant, whence these schemes reduce to the 4 stage Gauss-Legendre method. Another reduction to these methods is obtained, when $\alpha_0 = 0$. Then either $\mathbf{y}^{(2)} = \mathbf{y}^{(3)}$, $\mathbf{y}^{(4)} = \mathbf{y}^{(5)}$ (for $\tilde{c}_2 = \tilde{c}_3$) or $\mathbf{y}^{(2)} = \mathbf{y}^{(4)}$, $\mathbf{y}^{(3)} = \mathbf{y}^{(5)}$ (for $\tilde{c}_2 = -\tilde{c}_3$), and the scheme reduces to the four stages $\mathbf{y}^{(1)}$, $\mathbf{y}^{(2)}$, $\mathbf{y}^{(4)}$, $\mathbf{y}^{(5)}$ with weights $(b_1, b_2 + b_3, b_2 + b_3, b_1)$. Thus, this subsection provides a three parameter family of "6 stage deformations" of the 4 stage Gauss-Legendre method.

Order 10 : The quadrature conditions $\tilde{B}(9)$ are not consistent with the assumption $\tilde{c}_1^2 \neq \tilde{c}_2^2 = \tilde{c}_3^2$.

3.6.8 6 stages, $\tilde{c}_1^2 = \tilde{c}_2^2 = \tilde{c}_3^2$

A 4th order method is given by (3.23)/(3.24) subject to the constraints

$$b_1 + b_2 + b_3 = \frac{1}{2}, \quad \tilde{c}_1^2 = \tilde{c}_2^2 = \tilde{c}_3^2 = \frac{1}{12}.$$

Elimination of $b_3 = 1/2 - b_1 - b_2$, say, leaves an eight-parameter family of schemes. No order higher than 4 can be attained.

4 Classification of non-standard schemes through 6 stages

In section 3 self-adjointness (2.4) induced by the standard permutation $\sigma(i) = s + 1 - i$ was considered leading to Butcher parameters of the form (2.7). In this section we give a comprehensive account of the symplectic self-adjoint schemes through 6 stages associated with all other ("non-standard") permutations.

The standard families of methods are richer than those considered now. In particular, because of

$$\tilde{c}_i = -\tilde{c}_{\sigma(i)} = \tilde{c}_{\sigma(\sigma(i))} = \ldots$$

all non-standard permutations lead to self-adjoint methods featuring some degeneracy: several of the abscissae $\tilde{c}_i$ must coincide. Either there are several fixed points of σ, leading to vanishing abscissae, or there are cycles $(i, \sigma(i), \sigma(\sigma((i)), \ldots)$ of length > 2. Indeed, the standard permutation is distinguished by the fact, that all cycles are of length 2 apart from a single fixed point (for odd stage numbers).

Fortunately, for a complete classification of self-adjoint schemes not all permutations need to be considered. The constraints induced by a pair of conjugate permutations σ, σ' (i.e., $\sigma' = \alpha \circ \sigma \circ \alpha^{-1}$ with some permutation α) lead to Butcher parameters which are equivalent in the sense of definition 2.1:

Theorem 4.1 *Let $\mathcal{P}$ and $\mathcal{P}'$ be conjugate permutation matrices. To any self-adjoint scheme with parameters $S, \tilde{\mathbf{c}}, \mathbf{b}$ satisfying $S = -\mathcal{P} S \mathcal{P}^{-1}$, $\tilde{\mathbf{c}} = -\mathcal{P}\tilde{\mathbf{c}}$, $\mathbf{b} = \mathcal{P}\mathbf{b}$, there exists an equivalent set of parameters $S', \tilde{\mathbf{c}}', \mathbf{b}'$ satisfying $S' = -\mathcal{P}' S' \mathcal{P}'^{-1}$, $\tilde{\mathbf{c}}' = -\mathcal{P}'\tilde{\mathbf{c}}'$, $\mathbf{b}' = \mathcal{P}'\mathbf{b}'$.*

Proof Let $\mathcal{P}' = \mathcal{T}\mathcal{P}\mathcal{T}^{-1}$ with some permutation matrix $\mathcal{T}$. Then the Butcher parameters $S' = \mathcal{T}S\mathcal{T}^{-1}$, $\tilde{\mathbf{c}}' = \mathcal{T}\tilde{\mathbf{c}}$, $\mathbf{b}' = \mathcal{T}\mathbf{b}$ are equivalent to $S, \tilde{\mathbf{c}}, \mathbf{b}$ and satisfy the symmetry constraints (2.4) given by $\mathcal{P}'$. □

One concludes that for a complete classification of all symplectic self-adjoint schemes it is sufficient to choose one representative from each conjugacy class and classify all schemes satisfying (2.4) with this representative. Theorem 4.1 also holds, if some odd power of $\mathcal{P}$ is conjugate to $\mathcal{P}'$. If the group order of the permutation is odd, then the resulting schemes are equivalent to those associated with $\mathcal{P}' = I$, the identity matrix:

Theorem 4.2 *Any consistent self-adjoint scheme satisfying (2.4) with a permutation σ of odd group order reduces to the implicit midpoint rule of subsection 3.1.*

Proof The symmetry constraints (2.4) imply $S = (-1)^n \mathcal{P}^n S \mathcal{P}^{-n}$, where $\mathcal{P}$ is the matrix representation of σ. If n is the group order of σ, then $\mathcal{P}^n$ is the identity matrix and $S = -S$ for odd n, i.e., $S = 0$. With remark 2.2 the scheme may subsequently be reduced to the 1 stage method with $S = (s_{11}) = 0$, i.e., the implicit midpoint rule. □

In the following we classify the conjugacy classes via the cycle structure shared by their representatives. The corresponding background and notation is reviewed in the appendix.

4.1 1 stage

The implicit midpoint rule of subsection 3.1 is the only consistent self-adjoint method with 1 stage.

4.2 2 stages

There are 2 conjugacy classes in the symmetric group on $\{1, 2\}$:

conjugacy class	representative σ_{id}^{C}	group order
$C_1(2)$	$(1)(2)$	1
$C_2(2)$	$(1, 2)$	2

The scheme related to $C_1(2)$ reduces to the implicit midpoint rule of subsection 3.1. The representative $\sigma = (1, 2)$ of $C_2(2)$ leads to the schemes of subsection 3.2.

4.3 3 stages

There are 3 conjugacy classes in the symmetric group on $\{1, 2, 3\}$:

conjugacy class	representative σ_{id}^{C}	group order
$C_1(3)$	$(1)(2)(3)$	1
$C_2(3)$	$(1, 2)(3)$	2
$C_3(3)$	$(1, 2, 3)$	3

The schemes related to $C_1(3)$ and $C_3(3)$ reduce to the implicit midpoint rule of subsection 3.1. The representative $\sigma = (1,3)(2)$ of $C_2(3)$ leads to the schemes of subsection 3.3.

4.4 4 stages

There are 5 conjugacy classes in the symmetric group on $\{1,2,3,4\}$:

conjugacy class	representative σ_{id}^{C}	group order
$C_1(4)$	$(1)(2)(3)(4)$	1
$C_2(4)$	$(1,2)(3)(4)$	2
$C_3(4)$	$(1,2)(3,4)$	2
$C_4(4)$	$(1,2,3)(4)$	3
$C_5(4)$	$(1,2,3,4)$	4

4.4.1 4 stages, conjugacy classes $C_1(4), C_4(4), C_5(4)$

The schemes related to $C_1(4)$ and $C_4(4)$ reduce to the implicit midpoint rule of subsection 3.1. The constraints (2.4) induced by the representative $\sigma = (1,2,3,4)$ of $C_5(4)$ leads to symplectic self-adjoint schemes with parameters of the form

$$C_5(4): \qquad (s_{ij}) = \begin{pmatrix} 0 & s_{12} & 0 & s_{12} \\ -s_{12} & 0 & -s_{12} & 0 \\ 0 & s_{12} & 0 & s_{12} \\ -s_{12} & 0 & -s_{12} & 0 \end{pmatrix}.$$

According to remark 2.2 these schemes reduce to two stage methods due to coinciding rows.

4.4.2 4 stages, conjugacy class $C_2(4)$

The constraints (2.4) induced by the representative $\sigma = (1,4)(2)(3)$ of $C_2(4)$ lead to symplectic self-adjoint schemes with a Butcher tableau of the form

$$\begin{array}{c|cccc}
\frac{1}{2}+\tilde{c}_1 & \frac{b_1}{2} & \left(\frac{1}{2}+s_{12}\right)b_2 & \left(\frac{1}{2}+s_{13}\right)b_3 & \left(\frac{1}{2}+s_{14}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{12}\right)b_1 & \frac{b_2}{2} & \frac{b_3}{2} & \left(\frac{1}{2}+s_{12}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{13}\right)b_1 & \frac{b_2}{2} & \frac{b_3}{2} & \left(\frac{1}{2}+s_{13}\right)b_1 \\
\frac{1}{2}-\tilde{c}_1 & \left(\frac{1}{2}-s_{14}\right)b_1 & \left(\frac{1}{2}-s_{12}\right)b_2 & \left(\frac{1}{2}-s_{13}\right)b_3 & \frac{b_1}{2} \\
\hline
 & b_1 & b_2 & b_3 & b_1
\end{array}$$

with the row-sum conditions (2.3) implemented by $s_{14} = (\tilde{c}_1 - s_{12}\, b_2 - s_{13}\, b_3)/b_1$. It involves 6 free parameters $b_1, b_2, b_3,\ \tilde{c}_1,\ s_{12}, s_{13}$.

Order 2 is granted via the consistency condition $2\,b_1 + b_2 + b_3 = 1$.

Order 4 is granted via the two constraints $2\,b_1 + b_2 + b_3 = 1$ and $b_1\,\tilde{c}_1^2 = 1/24$ in $\tilde{B}(3)$.

Order 6 is attained by

$$b_1 = \frac{5}{18}\,, \quad b_2 + b_3 = \frac{4}{9}\,, \quad s_{12} = s_{13} = \frac{3\,\tilde{c}_1}{2}\,, \quad s_{14} = \frac{6\,\tilde{c}_1}{5}\,, \quad \tilde{c}_1^2 = \frac{3}{20}\,.$$

Since the second and the third row of the Butcher matrix coincide, the scheme reduces to 3 stages. It is equivalent to the Gauss-Legendre method of subsection 3.3.3.

Order 8 is not possible.

4.4.3 4 stages, conjugacy class $C_3(4)$

The representative $\sigma = (1,4)(2,3)$ of $C_3(4)$ leads to the schemes of subsection 3.4.

4.5 5 stages

There are 7 conjugacy classes in the symmetric group on $\{1,2,3,4,5\}$:

conjugacy class	representative σ_{id}^C	group order
$C_1(5)$	$(1)(2)(3)(4)(5)$	1
$C_2(5)$	$(1,2)(3)(4)(5)$	2
$C_3(5)$	$(1,2)(3,4)(5)$	2
$C_4(5)$	$(1,2,3)(4)(5)$	3
$C_5(5)$	$(1,2,3)(4,5)$	6
$C_6(5)$	$(1,2,3,4)(5)$	4
$C_7(5)$	$(1,2,3,4,5)$	5

4.5.1 5 stages, conjugacy classes $C_1(5), C_4(5), C_5(5), C_6(5), C_7(5)$

The schemes related to $C_1(5)$, $C_4(5)$ and $C_7(5)$ reduce to the implicit midpoint rule of subsection 3.1.

The constraints (2.4) induced by the representatives $(1,2,3)(4,5)$ of $C_5(5)$ and $(1,2,3,4)(5)$ of $C_6(5)$, respectively, lead to symplectic self-adjoint schemes with parameters of the form

$$C_5(5): \qquad (s_{ij}) = \begin{pmatrix} 0 & 0 & 0 & s_{14} & -s_{14} \\ 0 & 0 & 0 & s_{14} & -s_{14} \\ 0 & 0 & 0 & s_{14} & -s_{14} \\ -s_{14} & -s_{14} & -s_{14} & 0 & s_{45} \\ s_{14} & s_{14} & s_{14} & -s_{45} & 0 \end{pmatrix}$$

and

$$C_6(5): \qquad (s_{ij}) \;=\; \begin{pmatrix} 0 & s_{12} & 0 & s_{12} & s_{15} \\ -s_{12} & 0 & -s_{12} & 0 & -s_{15} \\ 0 & s_{12} & 0 & s_{12} & s_{15} \\ -s_{12} & 0 & -s_{12} & 0 & -s_{15} \\ -s_{15} & s_{15} & -s_{15} & s_{15} & 0 \end{pmatrix},$$

respectively. Due to coinciding rows these schemes reduce to 3 stage methods according to remark 2.2.

4.5.2 5 stages, conjugacy class $C_2(5)$

The constraints (2.4) induced by the representative $\sigma = (1,5)(2)(3)(4)$ of $C_2(5)$ leads to symplectic self-adjoint schemes with a Butcher tableau of the form

$$\begin{array}{c|ccccc}
\frac{1}{2}+\tilde{c}_1 & \frac{b_1}{2} & \left(\frac{1}{2}+s_{12}\right)b_2 & \left(\frac{1}{2}+s_{13}\right)b_3 & \left(\frac{1}{2}+s_{14}\right)b_4 & \left(\frac{1}{2}+s_{15}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{12}\right)b_1 & \frac{b_2}{2} & \frac{b_3}{2} & \frac{b_4}{2} & \left(\frac{1}{2}+s_{12}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{13}\right)b_1 & \frac{b_2}{2} & \frac{b_3}{2} & \frac{b_4}{2} & \left(\frac{1}{2}+s_{13}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{14}\right)b_1 & \frac{b_2}{2} & \frac{b_3}{2} & \frac{b_4}{2} & \left(\frac{1}{2}+s_{14}\right)b_1 \\
\frac{1}{2}-\tilde{c}_1 & \left(\frac{1}{2}-s_{15}\right)b_1 & \left(\frac{1}{2}-s_{12}\right)b_2 & \left(\frac{1}{2}-s_{13}\right)b_3 & \left(\frac{1}{2}-s_{14}\right)b_4 & \frac{b_1}{2} \\
\hline
 & b_1 & b_2 & b_3 & b_4 & b_1
\end{array}$$

(4.26)
with the row-sum conditions (2.3) implemented by

$$s_{15} \;=\; \frac{1}{b_1}\,(\,\tilde{c}_1 - s_{12}\,b_2 - s_{13}\,b_3 - s_{14}\,b_4\,)\;.$$

It involves 8 free parameters $b_1, b_2, b_3, b_4,\ \tilde{c}_1,\ s_{12},\ s_{13},\ s_{14}$.

Order 2 is granted via the consistency condition $2\,b_1 + b_2 + b_3 + b_4 = 1$.

Order 4 is granted via the two constraints $2\,b_1 + b_2 + b_3 + b_4 = 1$ and $b_1\,\tilde{c}_1^2 = 1/24$.

Order 6 fixes $b_1 = 5/18$ and $\tilde{c}_1^2 = 3/20$. Putting

$$s_{12} \;=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_2)\,, \quad s_{13} \;=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_3)\,, \quad s_{14} \;=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_4)$$

the order conditions simplify to the constraints

$$b_2 + b_3 + b_4 \;=\; \frac{4}{9}\,, \quad b_2\,\epsilon_2 + b_3\,\epsilon_3 + b_4\,\epsilon_4 \;=\; 0\,, \quad b_2\,\epsilon_2^2 + b_3\,\epsilon_3^2 + b_4\,\epsilon_4^2 \;=\; 0$$

implying $s_{15} = 6\,\tilde{c}_1/5$. We note that

$$\tilde{A}_i^{(2)} \;=\; \sum_{j=1}^{5} s_{ij}\,b_j\,\tilde{c}_j \;-\; \frac{\tilde{c}_i^2}{2} \;+\; \frac{1}{8} \;=\; \begin{cases} \frac{1}{8}\,\epsilon_i & \text{for } i = 2,3,4 \\ 0 & \text{for } i = 1,5 \end{cases}$$

whence the parameters ϵ_i represent the simplifying assumption $\tilde{A}(2)$, which is not necessarily satisfied in this case. We assume that $\epsilon_2, \epsilon_3, \epsilon_4$ are mutually distinct since otherwise several rows in (s_{ij}) coincide and the scheme reduces to a method with less stages. Solving the constraints for b_2, b_3, b_4 one obtains a family of 6th order schemes (4.26) with

$$\begin{aligned}
b_1 &= \frac{5}{18}\,, \qquad \tilde{c}_1^2 = \frac{3}{20}\,, & s_{15} &= \frac{6}{5}\,\tilde{c}_1\,, \\
b_2 &= \frac{4\,\epsilon_3\,\epsilon_4}{9\,(\epsilon_2-\epsilon_3)\,(\epsilon_2-\epsilon_4)}\,, & s_{12} &= \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_2)\,, \\
b_3 &= \frac{4\,\epsilon_2\,\epsilon_4}{9\,(\epsilon_3-\epsilon_2)\,(\epsilon_3-\epsilon_4)}\,, & s_{13} &= \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_3)\,, \\
b_4 &= \frac{4\,\epsilon_2\,\epsilon_3}{9\,(\epsilon_4-\epsilon_2)\,(\epsilon_4-\epsilon_3)}\,, & s_{14} &= \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_4)
\end{aligned}$$

involving three free parameters $\epsilon_2, \epsilon_3, \epsilon_4$.

Order 8 is not possible.

4.5.3 5 stages, conjugacy class $C_3(5)$

The constraints (2.4) induced by the representatives $(1,5)(2,4)(3)$ of $C_3(5)$ lead to the schemes of subsection 3.5.

4.6 6 stages

There are 11 conjugacy classes in the symmetric group on $\{1,2,3,4,5,6\}$:

conjugacy class	representative $\sigma_{\rm id}^C$	group order
$C_1(6)$	$(1)(2)(3)(4)(5)(6)$	1
$C_2(6)$	$(1,2)(3)(4)(5)(6)$	2
$C_3(6)$	$(1,2)(3,4)(5)(6)$	2
$C_4(6)$	$(1,2)(3,4)(5,6)$	2
$C_5(6)$	$(1,2,3)(4)(5)(6)$	3
$C_6(6)$	$(1,2,3)(4,5)(6)$	6
$C_7(6)$	$(1,2,3)(4,5,6)$	3
$C_8(6)$	$(1,2,3,4)(5)(6)$	4
$C_9(6)$	$(1,2,3,4)(5,6)$	4
$C_{10}(6)$	$(1,2,3,4,5)(6)$	5
$C_{11}(6)$	$(1,2,3,4,5,6)$	6

4.6.1 6 stages, conjugacy classes $C_1(6), C_5(6), C_7(6), \ldots, C_{11}(6)$

The schemes related to $C_1(6)$, $C_5(6)$, $C_7(6)$ and $C_{10}(6)$ reduce to the implicit midpoint rule of subsection 3.1. The constraints (2.4) induced by the representatives $(1,2,3)(4,5)(6)$ of $C_6(6)$, $(1,2,3,4)(5)(6)$ of $C_8(6)$, and $(1,2,3,4)(5,6)$ of $C_9(6)$, respectively, lead to symplectic self-adjoint schemes with parameters of the form

$$C_6(6): \qquad (s_{ij}) \;=\; \begin{pmatrix} 0 & 0 & 0 & s_{14} & -s_{14} & 0 \\ 0 & 0 & 0 & s_{14} & -s_{14} & 0 \\ 0 & 0 & 0 & s_{14} & -s_{14} & 0 \\ -s_{14} & -s_{14} & -s_{14} & 0 & s_{45} & s_{46} \\ s_{14} & s_{14} & s_{14} & -s_{45} & 0 & -s_{46} \\ 0 & 0 & 0 & -s_{46} & s_{46} & 0 \end{pmatrix},$$

$$C_8(6): \qquad (s_{ij}) \;=\; \begin{pmatrix} 0 & s_{12} & 0 & s_{12} & s_{15} & s_{16} \\ -s_{12} & 0 & -s_{12} & 0 & -s_{15} & -s_{16} \\ 0 & s_{12} & 0 & s_{12} & s_{15} & s_{16} \\ -s_{12} & 0 & -s_{12} & 0 & -s_{15} & -s_{16} \\ -s_{15} & s_{15} & -s_{15} & s_{15} & 0 & 0 \\ -s_{16} & s_{16} & -s_{16} & s_{16} & 0 & 0 \end{pmatrix},$$

and

$$C_9(6): \qquad (s_{ij}) \;=\; \begin{pmatrix} 0 & s_{12} & 0 & s_{12} & s_{15} & s_{16} \\ -s_{12} & 0 & -s_{12} & 0 & -s_{16} & -s_{15} \\ 0 & s_{12} & 0 & s_{12} & s_{15} & s_{16} \\ -s_{12} & 0 & -s_{12} & 0 & -s_{16} & -s_{15} \\ -s_{15} & s_{16} & -s_{16} & s_{16} & 0 & s_{56} \\ -s_{16} & s_{15} & -s_{15} & s_{15} & -s_{56} & 0 \end{pmatrix},$$

respectively. According to remark 2.2, in all cases the schemes reduce to 4 stage methods due to coinciding rows.

The constraints (2.4) induced by the representative $(1,2,3,4,5,6)$ of $C_{11}(6)$ lead to symplectic self-adjoint schemes with parameters of the form

$$C_{11}(6): \qquad (s_{ij}) \;=\; \begin{pmatrix} 0 & s_{12} & s_{13} & s_{14} & -s_{13} & s_{12} \\ -s_{12} & 0 & -s_{12} & -s_{13} & -s_{14} & s_{13} \\ -s_{13} & s_{12} & 0 & s_{12} & s_{13} & s_{14} \\ -s_{14} & s_{13} & -s_{12} & 0 & -s_{12} & -s_{13} \\ s_{13} & s_{14} & -s_{13} & s_{12} & 0 & s_{12} \\ -s_{12} & -s_{13} & -s_{14} & s_{13} & -s_{12} & 0 \end{pmatrix},$$

weights $b_1 = b_2 = \ldots = b_6$ and abscissae $\tilde{c}_1 = \tilde{c}_3 = \tilde{c}_5 = -\tilde{c}_2 = -\tilde{c}_4 = -\tilde{c}_6$. We note that these schemes reduce to two stages, as some internal stages in (2.1) coincide:

$$\mathbf{y}^{(1)} = \mathbf{y}^{(3)} = \mathbf{y}^{(5)} := \tilde{\mathbf{y}}^{(1)}\,, \quad \mathbf{y}^{(2)} = \mathbf{y}^{(4)} = \mathbf{y}^{(6)} := \tilde{\mathbf{y}}^{(2)}\,,$$

where $\tilde{\mathbf{y}}^{(1)}, \tilde{\mathbf{y}}^{(2)}$ are the internal stages of the method

$$\begin{aligned} \tilde{\mathbf{y}}^{(1)} &= \mathbf{y}_n + h\left(\tilde{a}_{11}\mathbf{f}\left(t_n + \left(\tfrac{1}{2}+\tilde{c}_1\right)h, \tilde{\mathbf{y}}^{(1)}\right) + \tilde{a}_{12}\mathbf{f}\left(t_n + \left(\tfrac{1}{2}-\tilde{c}_1\right)h, \tilde{\mathbf{y}}^{(2)}\right)\right)\,, \\ \tilde{\mathbf{y}}^{(2)} &= \mathbf{y}_n + h\left(\tilde{a}_{21}\mathbf{f}\left(t_n + \left(\tfrac{1}{2}-\tilde{c}_1\right)h, \tilde{\mathbf{y}}^{(1)}\right) + \tilde{a}_{22}\mathbf{f}\left(t_n + \left(\tfrac{1}{2}-\tilde{c}_1\right)h, \tilde{\mathbf{y}}^{(2)}\right)\right)\,, \\ \mathbf{y}_{n+1} &= \mathbf{y}_n + h\,\tilde{b}\left(\mathbf{f}\left(t_n + \left(\tfrac{1}{2}+\tilde{c}_1\right)h, \tilde{\mathbf{y}}^{(1)}\right) + \mathbf{f}\left(t_n + \left(\tfrac{1}{2}-\tilde{c}_1\right)h, \tilde{\mathbf{y}}^{(2)}\right)\right) \end{aligned}$$

with

$$\tilde{b} = 3\,b_1\,, \quad \tilde{a}_{11} = \tilde{a}_{22} = \frac{\tilde{b}}{2}\,, \quad \tilde{a}_{12} = \left(\frac{1}{2} + \frac{2\,s_{12}+s_{14}}{3}\right)\tilde{b}\,, \quad \tilde{a}_{21} = \left(\frac{1}{2} - \frac{2\,s_{12}+s_{14}}{3}\right)\tilde{b}\,.$$

4.6.2 6 stages, conjugacy class $C_2(6)$

The constraints (2.4) induced by the representative $\sigma = (1,6)(2)(3)(4)(5)$ of $C_2(6)$ leads to symplectic self-adjoint schemes with a Butcher tableau of the form

$$\begin{array}{c|cccccc}
\frac{1}{2}+\tilde{c}_1 & \frac{b_1}{2} & \left(\frac{1}{2}+s_{12}\right)b_2 & \left(\frac{1}{2}+s_{13}\right)b_3 & \left(\frac{1}{2}+s_{14}\right)b_4 & \left(\frac{1}{2}+s_{15}\right)b_5 & \left(\frac{1}{2}+s_{16}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{12}\right)b_1 & \frac{b_2}{2} & \frac{b_3}{2} & \frac{b_4}{2} & \frac{b_5}{2} & \left(\frac{1}{2}+s_{12}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{13}\right)b_1 & \frac{b_2}{2} & \frac{b_3}{2} & \frac{b_4}{2} & \frac{b_5}{2} & \left(\frac{1}{2}+s_{13}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{14}\right)b_1 & \frac{b_2}{2} & \frac{b_3}{2} & \frac{b_4}{2} & \frac{b_5}{2} & \left(\frac{1}{2}+s_{14}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{15}\right)b_1 & \frac{b_2}{2} & \frac{b_3}{2} & \frac{b_4}{2} & \frac{b_5}{2} & \left(\frac{1}{2}+s_{15}\right)b_5 \\
\frac{1}{2}-\tilde{c}_1 & \left(\frac{1}{2}-s_{16}\right)b_1 & \left(\frac{1}{2}-s_{12}\right)b_2 & \left(\frac{1}{2}-s_{13}\right)b_3 & \left(\frac{1}{2}-s_{14}\right)b_4 & \left(\frac{1}{2}-s_{15}\right)b_5 & \frac{b_1}{2} \\
\hline
 & b_1 & b_2 & b_3 & b_4 & b_5 & b_1
\end{array}$$

(4.27)

with the row-sum conditions (2.3) implemented by

$$s_{16} \;=\; \frac{1}{b_1}\,(\,\tilde{c}_1 - s_{12}\,b_2 - s_{13}\,b_3 - s_{14}\,b_4 - s_{15}\,b_5\,)\;.$$

It involves 10 free parameters $b_1, b_2, b_3, b_4, b_5,\ \tilde{c}_1,\ s_{12}, s_{13}, s_{14}, s_{15}$.

Order 2 is granted via the consistency condition $2\,b_1 + b_2 + b_3 + b_4 + b_5 = 1$.

Order 4 is granted via the two constraints $2\,b_1 + b_2 + b_3 + b_4 + b_5 = 1$ and $b_1\,\tilde{c}_1^2 = 1/24$.

Order 6 fixes $b_1 = 5/18$ and $\tilde{c}_1^2 = 3/20$. Putting

$$s_{12} \;=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_2)\;,\;\; s_{13} \;=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_3)\;,\;\; s_{14} \;=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_4)\;,\;\; s_{15} \;=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_5)$$

the order conditions simplify to the constraints

$$b_2 + b_3 + b_4 + b_5 \;=\; \frac{4}{9}\;,\;\; b_2\,\epsilon_2 + b_3\,\epsilon_3 + b_4\,\epsilon_4 + b_5\,\epsilon_5 \;=\; 0\;,\;\; b_2\,\epsilon_2^2 + b_3\,\epsilon_3^2 + b_4\,\epsilon_4^2 + b_5\,\epsilon_5^2 \;=\; 0$$

implying $s_{16} = 6\,\tilde{c}_1/5$. We note that

$$\tilde{A}_i^{(2)} \;=\; \sum_{j=1}^{5} s_{ij}\,b_j\,\tilde{c}_j \;-\; \frac{\tilde{c}_i^2}{2} \;+\; \frac{1}{8} \;=\; \begin{cases} \frac{1}{8}\,\epsilon_i & \text{for } i = 2,3,4 \\ 0 & \text{for } i = 1,5 \end{cases}$$

whence the parameters ϵ_i represent the simplifying assumption $\tilde{A}(2)$, which is not necessarily satisfied in this case. We assume that $\epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5$ are mutually distinct since otherwise several rows in (s_{ij}) coincide and the scheme reduces to a method with less stages. Solving the constraints for b_2, b_3, b_4 one obtains a family of 6th order schemes (4.26) with

$$\begin{aligned}
b_1 \;&=\; \frac{5}{18}\;,\quad b_2 \;=\; \frac{4\,\epsilon_3\epsilon_4 - 9\,(\epsilon_5-\epsilon_3)\,(\epsilon_5-\epsilon_4)\,b_5}{9\,(\epsilon_2-\epsilon_3)\,(\epsilon_2-\epsilon_4)}\;,\\
b_3 \;&=\; \frac{4\,\epsilon_2\epsilon_4 - 9\,(\epsilon_5-\epsilon_2)\,(\epsilon_5-\epsilon_4)\,b_5}{9\,(\epsilon_3-\epsilon_2)\,(\epsilon_3-\epsilon_4)}\;,\quad b_4 \;=\; \frac{4\,\epsilon_2\epsilon_3 - 9\,(\epsilon_5-\epsilon_4)\,(\epsilon_5-\epsilon_3)\,b_5}{9\,(\epsilon_4-\epsilon_2)\,(\epsilon_4-\epsilon_3)}\;,\\
s_{12} \;&=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_2)\;,\quad s_{13} \;=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_3)\;,\quad s_{14} \;=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_4)\;,\\
s_{15} \;&=\; \frac{3}{2}\,\tilde{c}_1\,(1-\epsilon_5)\;,\quad s_{16} \;=\; \frac{6}{5}\,\tilde{c}_1\;,\quad \tilde{c}_1^2 \;=\; \frac{3}{20}
\end{aligned}$$

involving five free parameters $b_5, \epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5$.

Order 8 is not possible.

4.6.3 6 stages, conjugacy class $C_3(6)$

The constraints (2.4) induced by the representative $\sigma = (1,6)(2,5)(3)(4)$ of $C_3(6)$ leads to symplectic self-adjoint schemes with a Butcher tableau of the form

$$\begin{array}{c|cccccc}
\frac{1}{2}+\tilde{c}_1 & \frac{b_1}{2} & \left(\frac{1}{2}+s_{12}\right)b_2 & \left(\frac{1}{2}+s_{13}\right)b_3 & \left(\frac{1}{2}+s_{14}\right)b_4 & \left(\frac{1}{2}+s_{15}\right)b_2 & \left(\frac{1}{2}+s_{16}\right)b_1 \\
\frac{1}{2}+\tilde{c}_2 & \left(\frac{1}{2}-s_{12}\right)b_1 & \frac{b_2}{2} & \left(\frac{1}{2}+s_{23}\right)b_3 & \left(\frac{1}{2}+s_{24}\right)b_4 & \left(\frac{1}{2}+s_{25}\right)b_2 & \left(\frac{1}{2}+s_{15}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{13}\right)b_1 & \left(\frac{1}{2}-s_{23}\right)b_2 & \frac{b_3}{2} & \frac{b_4}{2} & \left(\frac{1}{2}+s_{23}\right)b_2 & \left(\frac{1}{2}+s_{13}\right)b_1 \\
\frac{1}{2} & \left(\frac{1}{2}-s_{14}\right)b_1 & \left(\frac{1}{2}-s_{24}\right)b_2 & \frac{b_3}{2} & \frac{b_4}{2} & \left(\frac{1}{2}+s_{24}\right)b_2 & \left(\frac{1}{2}+s_{14}\right)b_1 \\
\frac{1}{2}-\tilde{c}_2 & \left(\frac{1}{2}-s_{15}\right)b_1 & \left(\frac{1}{2}-s_{25}\right)b_2 & \left(\frac{1}{2}-s_{23}\right)b_3 & \left(\frac{1}{2}-s_{24}\right)b_4 & \frac{b_2}{2} & \left(\frac{1}{2}+s_{12}\right)b_1 \\
\frac{1}{2}-\tilde{c}_1 & \left(\frac{1}{2}-s_{16}\right)b_1 & \left(\frac{1}{2}-s_{15}\right)b_2 & \left(\frac{1}{2}-s_{13}\right)b_3 & \left(\frac{1}{2}-s_{14}\right)b_4 & \left(\frac{1}{2}-s_{12}\right)b_2 & \frac{b_1}{2} \\
\hline
 & b_1 & b_2 & b_3 & b_4 & b_2 & b_1
\end{array}$$

(4.28)

with the row-sum conditions (2.3) implemented by

$$\begin{aligned}
s_{16} &= \frac{1}{b_1}\left(\tilde{c}_1 - s_{12}\,b_2 - s_{13}\,b_3 - s_{14}\,b_4 - s_{15}\,b_2\right), \\
s_{25} &= \frac{1}{b_2}\left(\tilde{c}_2 + s_{12}\,b_1 - s_{23}\,b_3 - s_{24}\,b_4 - s_{15}\,b_1\right).
\end{aligned}$$

It involves 12 free parameters $b_1, b_2, b_3, b_4,\ \tilde{c}_1, \tilde{c}_2,\ s_{12}, s_{13}, s_{14}, s_{15}, s_{23}, s_{24}$.

Order 2 is granted via the consistency condition $2\,(b_1+b_2)+b_3+b_4+b_5 = 1$.

Order 4 is granted via the two constraints $\tilde{B}(3)$:

$$2\,(b_1+b_2)+b_3+b_4+b_5 \;=\; 1\;, \quad b_1\,\tilde{c}_1^2 + b_2\,\tilde{c}_2^2 \;=\; \frac{1}{24}\;.$$

Order 6 imposes 5 equations. We parametrize the six independent entries of the Butcher matrix

$$
\begin{aligned}
s_{13} &= \tilde{c}_1 \left(\frac{3}{2} - 12\,\epsilon_3\right) + \beta\, b_2\, \tilde{c}_2 \;, \quad s_{14} \;=\; \tilde{c}_1 \left(\frac{3}{2} - 12\,\epsilon_4\right) + \gamma\, b_2\, \tilde{c}_2 \;, \\
s_{23} &= \tilde{c}_2 \left(\frac{3}{2} - 12\,\epsilon_3\right) - \beta\, b_1\, \tilde{c}_1 \;, \quad s_{24} \;=\; \tilde{c}_2 \left(\frac{3}{2} - 12\,\epsilon_4\right) - \gamma\, b_1\, \tilde{c}_1 \;, \\
s_{16} &= \tilde{c}_1 (3 - 12\,\tilde{c}_1^2) \;+\; 2\,\delta\, b_2^2\, \tilde{c}_2 \;-\; 24\, b_2\, \tilde{c}_1\, \tilde{c}_2 \Big(\epsilon_0\, \tilde{c}_2 + (\beta\, b_3 + \gamma\, b_4)\, \tilde{c}_1\Big) \;, \\
s_{25} &= \tilde{c}_2 (3 - 12\,\tilde{c}_2^2) \;+\; 2\,\delta\, b_1^2\, \tilde{c}_1 \;+\; 24\, b_1\, \tilde{c}_1\, \tilde{c}_2 \Big(\epsilon_0\, \tilde{c}_1 + (\beta\, b_3 + \gamma\, b_4)\, \tilde{c}_2\Big) \;, \\
s_{12} &= (\tilde{c}_1 - \tilde{c}_2) \left(\frac{3}{2} + 6\, \tilde{c}_1\, \tilde{c}_2 + \delta\, b_1\, b_2\right) \;+\; 12\,(b_1\, \tilde{c}_1^3 + b_2\, \tilde{c}_2^3)\,(\epsilon_0 - \beta\, b_3 - \gamma\, b_4) \;, \\
s_{15} &= (\tilde{c}_1 + \tilde{c}_2) \left(\frac{3}{2} - 6\, \tilde{c}_1\, \tilde{c}_2 - \delta\, b_1\, b_2\right) \;+\; 12\,(b_1\, \tilde{c}_1^3 - b_2\, \tilde{c}_2^3)\,(\epsilon_0 + \beta\, b_3 + \gamma\, b_4)
\end{aligned}
$$

by new parameters $\beta, \gamma, \delta, \epsilon_0, \epsilon_3, \epsilon_4$. We note that the Jacobi determinant

$$
\frac{\partial\,(s_{12}, s_{13}, s_{14}, s_{15}, s_{23}, s_{24})}{\partial\,(\beta, \gamma, \delta, \epsilon_0, \epsilon_3, \epsilon_4)} \;=\; 3456\; b_1\, b_2\, (b_1\, \tilde{c}_1^2 + b_2 \tilde{c}_2^2)^2\, (b_1 \tilde{c}_1^4 + b_2\, \tilde{c}_4^4)
$$

simplifies to $\frac{3}{80}\, b_1\, b_2 \neq 0$ due to the quadrature conditions $\tilde{B}(5)$:

$$
2\,(b_1 + b_2) + b_3 + b_4 \;=\; 1 \;, \quad b_1\, \tilde{c}_1^2 + b_2\, \tilde{c}_2^2 \;=\; \frac{1}{24} \;, \quad b_1\, \tilde{c}_1^4 + b_2\, \tilde{c}_2^4 \;=\; \frac{1}{160} \;.
$$

Order 6 is attained via the two further constraints

$$
2\, b_1\, b_2\, (\tilde{c}_1^2 - \tilde{c}_2^2)\, \epsilon_0 \;=\; b_3\, \epsilon_3 + b_4\, \epsilon_4 \;, \quad b_1\, b_2\, \epsilon_0^2 \;=\; -\, 80\, (\, b_3\, \epsilon_3^2 + b_4\, \epsilon_4^2\,) \;. \tag{4.29}
$$

We note that with

$$
\tilde{A}_i^{(2)} \;=\; \sum_{j=1}^{6} s_{ij}\, b_j\, \tilde{c}_j \;-\; \frac{\tilde{c}_i^2}{2} \;+\; \frac{1}{8} \;=\; \begin{cases} b_2\, \tilde{c}_2^2\, \epsilon_0 & , \quad i = 1, 6 \\ -b_1\, \tilde{c}_1^2\, \epsilon_0 & , \quad i = 2, 5 \\ \epsilon_i & , \quad i = 3, 4 \end{cases}
$$

the parameters $\epsilon_0, \epsilon_3, \epsilon_4$ represent the simplifying assumption $\tilde{A}(2)$, which is not necessarily satisfied.

Order 8: The quadrature conditions $\tilde{B}(7)$ imply $b_1\, b_2\, \tilde{c}_1^2\, \tilde{c}_2^2\, (\tilde{c}_1^2 - \tilde{c}_2^2)^2 = 1/13440$, whence $\tilde{c}_1^2, \tilde{c}_2^2$ are mutually distinct and non-zero. Further, one finds

$$
\epsilon \;=\; 0 \;, \quad \delta \;=\; \frac{1}{b_1\, b_2} \left(4\, \tilde{c}_1\, \tilde{c}_2 \;+\; \frac{3}{40}\, \frac{\beta\, b_3 + \gamma\, b_4}{\tilde{c}_1^2 - \tilde{c}_2^2} \right).
$$

From the constraints (4.29) one concludes $\epsilon_3 = \epsilon_4$ for non-zero b_3, b_4.

Case $\epsilon_3 = \epsilon_4 = 0$**:** The quadrature conditions $\tilde{B}(7)$ lead to

$$b_1 \;=\; \frac{3-20\tilde{c}_2^2}{480\,\tilde{c}_1^2\,(\tilde{c}_1^2-\tilde{c}_2^2)}\;, \quad b_2 \;=\; \frac{3-20\tilde{c}_1^2}{480\,\tilde{c}_2^2\,(\tilde{c}_2^2-\tilde{c}_1^2)}\;, \quad b_3+b_4 \;=\; \frac{4}{9}-\frac{1}{420\,\tilde{c}_1^2\tilde{c}_2^2}\;,$$

where $\tilde{c}_1, \tilde{c}_2$ are subject to the constraint

$$(3-20\,\tilde{c}_1^2)\,(3-20\,\tilde{c}_2^2) \;=\; -\frac{12}{7}\;. \tag{4.30}$$

The Butcher matrix is given by

$$\begin{aligned}
s_{13} &= \frac{3}{2}\,\tilde{c}_1+\beta\,b_2\,\tilde{c}_2\;, \quad s_{14} \;=\; \frac{3}{2}\,\tilde{c}_1+\gamma\,b_2\,\tilde{c}_2\;,\\
s_{23} &= \frac{3}{2}\,\tilde{c}_2-\beta\,b_1\,\tilde{c}_1\;, \quad s_{24} \;=\; \frac{3}{2}\,\tilde{c}_2-\gamma\,b_1\,\tilde{c}_1\;,\\
s_{16} &= \tilde{c}_1\left(3-20\,\tilde{c}_1^2+\frac{1}{3\,b_1}\right)+\frac{b_2\,\tilde{c}_2^3\,(\beta\,b_3+\gamma\,b_4)}{b_1\,(\tilde{c}_1^2-\tilde{c}_2^2)}\;,\\
s_{25} &= \tilde{c}_2\left(3-20\,\tilde{c}_2^2+\frac{1}{3\,b_2}\right)+\frac{b_1\,\tilde{c}_1^3\,(\beta\,b_3+\gamma\,b_4)}{b_2\,(\tilde{c}_1^2-\tilde{c}_2^2)}\;,\\
s_{12} &= (\tilde{c}_1-\tilde{c}_2)\left(\frac{3}{2}+\tilde{c}_1\,\tilde{c}_2\left(10-\frac{\beta\,b_3+\gamma\,b_4}{2\,(\tilde{c}_1^2-\tilde{c}_2^2)}\right)\right)\;,\\
s_{15} &= (\tilde{c}_1+\tilde{c}_2)\left(\frac{3}{2}-\tilde{c}_1\,\tilde{c}_2\left(10+\frac{\beta\,b_3+\gamma\,b_4}{2\,(\tilde{c}_1^2-\tilde{c}_2^2)}\right)\right)\;.
\end{aligned}$$

These methods are "6 stage deformations" of the 5 stage schemes of subsection 3.5.8, which are obtained after combining the third and fourth of the internal stages for $\beta = \gamma$.

Case $\epsilon_3 = \epsilon_4 \neq 0$**:** The constraints (4.29) imply $b_3 + b_4 = 0$, whence $\tilde{B}(7)$ leads to

$$b_1 = \frac{7\,(3+20\,\tilde{c}_2^2)}{144}\;, \quad b_2 = \frac{7\,(3+20\,\tilde{c}_1^2)}{144}\;, \quad b_3+b_4 \;= 0$$

and the constraints

$$560\,\tilde{c}_1^4-120\,\tilde{c}_1^2+3 \;=\; 0\;, \quad \tilde{c}_1^2+\tilde{c}_2^2 \;=\; \frac{3}{14}\;.$$

Other order conditions imply $\gamma = \beta$, $\delta = 3456\,\tilde{c}_1\tilde{c}_2/49$, leading to a Butcher matrix given by

$$s_{13} = s_{14} = \tilde{c}_1\left(\frac{3}{2}-12\,\epsilon_3\right)+\beta\,b_2\,\tilde{c}_2\;, \quad s_{23} = s_{24} = \tilde{c}_2\left(\frac{3}{2}-12\,\epsilon_3\right)-\beta\,b_1\,\tilde{c}_1\;,$$

$$s_{12} = (\tilde{c}_1-\tilde{c}_2)\left(\frac{3}{2}+10\,\tilde{c}_1\,\tilde{c}_2\right)\;, \quad s_{16} = \frac{\tilde{c}_1\,(27-100\,\tilde{c}_1^2)}{7}\;,$$

$$s_{15} = (\tilde{c}_1 + \tilde{c}_2) \left(\frac{3}{2} - 10\, \tilde{c}_1\, \tilde{c}_2 \right) , \quad s_{25} = \frac{\tilde{c}_2\, (27 - 100\, \tilde{c}_2^2)}{7} .$$

As the third and the fourth row in (s_{ij}) coincide the corresponding stages may be combined to a single stage with vanishing weight $b_3 + b_4$. Thus, this scheme is equivalent to the 4 stage Gauss-Legendre method.

Order 10 fixes $\delta = -3200\, \tilde{c}_1 \tilde{c}_2 / 189$ and $\beta = \gamma = -210\, \tilde{c}_1 \tilde{c}_2\, (\tilde{c}_1^2 - \tilde{c}_2^2)$. The quadrature conditions $\tilde{B}(9)$ lead to

$$b_1 \;=\; \frac{7\,(3 + 52\, \tilde{c}_2^2)}{400} , \quad b_2 \;=\; \frac{7\,(3 + 52\, \tilde{c}_1^2)}{400} , \quad b_3 + b_4 \;=\; \frac{32}{225}$$

and the constraints

$$1008\, \tilde{c}_1^2 - 280\, \tilde{c}_1^2 + 15 \;=\; 0 , \quad \tilde{c}_1^2 + \tilde{c}_2^2 \;=\; \frac{5}{18} .$$

With

$$s_{12} = \frac{5}{18} (\tilde{c}_1 - \tilde{c}_2)\; (7 + 36\, \tilde{c}_1\, \tilde{c}_2) \;,\; s_{13} = s_{14} = \frac{5}{16}\, \tilde{c}_1\, (9 - 28\, \tilde{c}_1^2) ,\; s_{16} = \frac{5}{81}\, \tilde{c}_1\, (33 - 76\, \tilde{c}_1^2) \;,$$
$$s_{15} = \frac{5}{18} (\tilde{c}_1 + \tilde{c}_2)\; (7 - 36\, \tilde{c}_1\, \tilde{c}_2) \;,\; s_{23} = s_{24} = \frac{5}{16}\, \tilde{c}_2\, (9 - 28\, \tilde{c}_2^2) ,\; s_{25} = \frac{5}{81}\, \tilde{c}_2\, (33 - 76\, \tilde{c}_2^2)$$

this scheme is equivalent to the 5 stage Gauss-Legendre method after combining the third and the fourth stage.

4.6.4 6 stages, conjugacy class $C_4(6)$

The representative $\sigma = (1,6)(2,5)(3,4)$ of $C_4(6)$ leads to the schemes of subsection 3.6.

5 Algebraically stable methods

Non-linear stability is a desirable property of a numerical method for solving a dissipative system of ordinary differential equations. A simple algebraic condition, closely related to symplecticity, can be shown to imply non-linear stability (see for example [17] and the references therein). A Runge-Kutta method is said to be *algebraically stable* if:

$$(5.31) \qquad b_i\, a_{ij} + b_j\, a_{ji} + b_i\, b_j \geq 0, \quad b_i \geq 0 \quad i, j = 1, \ldots, s.$$

Comparison of (2.5) and (5.31) immediately affirms that they have non-empty intersection: symplectic schemes with non-negative weights are algebraically stable.

The structure of Hamiltonian systems rules out many of the considerations which motivate the construction of numerical methods for dissipative systems. However, there are reasons why we may wish to investigate methods which are both symplectic and algebraically stable. One possible motivation might be to develop a single general purpose numerical integration method which has desirable properties when applied to either Hamiltonian or to dissipative systems. Although the maximal order Gauss-Legendre methods fall into this category, they can be expensive to implement since the implicit equations one has to solve at each time step are highly coupled. Iserles derived symplectic schemes which should be more efficient because they uncouple the non-linear equations [8]. However, those schemes fail to satisfy algebraic stability.

We may also wish to investigate algebraically stable methods in their own right, or methods possessing variants of algebraic stability. Common classifications, such as those derived using W-transforms [6], form only a subset of possible methods and our schemes could be viewed as another sub-class. Since our main interest here is the construction of symplectic Runge-Kutta methods, we do not pursue the issue of algebraic stability further to see if any interesting schemes exist. We shall however now illustrate that it is often quite straightforward to derive such methods from our classification.

Consider the 4 stage 6th order methods of subsection 3.4.3 with

$$b_1 \;=\; \frac{1}{24}\,\frac{1-12\,\tilde{c}_2^2}{\tilde{c}_1^2-\tilde{c}_2^2}\;, \quad b_2 \;=\; \frac{1}{24}\,\frac{1-12\,\tilde{c}_1^2}{\tilde{c}_2^2-\tilde{c}_1^2}\;, \quad b_1\,b_2\,(\tilde{c}_1^2-\tilde{c}_2^2)^2 \;=\; \frac{1}{720}\;,$$

implying the constraint (3.16) between $\tilde{c}_1$ and $\tilde{c}_2$. Real solutions exist, if $\tilde{c}_1^2 < 1/12$ or $\tilde{c}_1^2 > 3/20$, whence

$$c_2^2 \;=\; \frac{1}{12} \;-\; \frac{1}{15\,(12\,\tilde{c}_1^2-1)} \;>0\;.$$

Clearly both weights b_1, b_2 have to have the same sign. The contradictions

$$b_1<0\;,\; b_2<0\;,\; \tilde{c}_2^2<\tilde{c}_1^2 \quad\Longrightarrow\quad \tilde{c}_1^2<\frac{1}{12}<\tilde{c}_2^2\;,$$

$$b_1<0\;,\; b_2<0\;,\; \tilde{c}_1^2<\tilde{c}_2^2 \quad\Longrightarrow\quad \tilde{c}_2^2<\frac{1}{12}<\tilde{c}_1^2$$

rule out negative weights, whence *all* methods of the two-parameter family presented in subsection 3.4.3 are algebraically stable.

6 Conclusions

We have presented a complete classification of self-adjoint symplectic Runge-Kutta methods through 6 stages. This was made possible because for most of these schemes the simplifying assumptions turned out to be necessary and could in turn be used to eliminate any non-linearity beyond quadrature conditions from the order equations. The same procedure as outlined here can be used at higher stages. However, the necessity of simplifying assumptions as given in corollary 2.6 is not granted for 7 stages and above: there is some loss of generality in adopting simplifying assumptions to eliminate non-linear constraints. The loss of free parameters between the most general solution for a given order and the sub-family obtained by our construction will increase with growing stage numbers.

In contrast to most categorizations, and as a measure of the generality, the schemes presented here are not necessarily real-valued and are not constrained to any particular precision.

As yet, no numerical experiments have been carried out with the newly found methods. It is an open question as to which special cases of the multi-parameter families lead to schemes of practical interest. However, the complete classification presented here provides the basis for future research in the design of symplectic integrators of Runge-Kutta type.

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Appendix

We review some standard notation from the representation theory of symmetric groups used in section 4 (see, e.g., [12]).

Definition A.1 *A* **cycle structure** $C = (i_1, \ldots, i_{k-1})$ *on* $X = \{1, \ldots, s\}$ *is a family of indices*

$$0 =: i_0 < i_1 < i_2 < \ldots < i_{k-1} < i_k := s$$

such that $i_p - i_{p-1} \geq i_{p+1} - i_p$ *for all* $p = 1, \ldots, k-1$.

The indices of a cycle structure correspond to disjoint cycles

$$(i_{p-1}+1, i_{p-1}+2, \ldots, i_p) \mapsto (i_{p-1}+2, \ldots, i_p, i_{p-1}+1) \ , \quad p = 1, \ldots, k$$

fixing the remaining elements in $X \setminus \{i_{p-1}+1, \ldots, i_p\}$. The length (group order) $i_p - i_{p-1}$ of these cycles decreases with p. We rearrange the ordering of the elements in X by a permutation α and define the product of the disjoint cycles induced by C as follows:

Definition A.2 *Let $C = (i_1, \ldots, i_{k-1})$ be a cycle structure on $X = \{1, \ldots, s\}$, let $\alpha : X \mapsto X$ be a permutation. With*

$$\sigma_\alpha^C := \Big(\alpha(1), \ldots, \alpha(i_1)\Big) \Big(\alpha(i_1+1), \ldots, \alpha(i_2)\Big) \cdots \Big(\alpha(i_{k-1}+1), \ldots, \alpha(i_k)\Big)$$

one denotes the permutation $\sigma_\alpha^C : X \mapsto X$ given by

$$\begin{cases} \sigma_\alpha^C(\alpha(i_p)) = \alpha(i_{p-1}+1) \ , & p = 1, \ldots, k \ , \\ \sigma_\alpha^C(\alpha(j)) = \alpha(j+1) \ , & j \in X \setminus \{i_1, \ldots, i_k\} \ . \end{cases}$$

For example, on $X = \{1, \ldots, 8\}$ the permutation $\sigma = (1,4,7)(2,3)(5,8)(6)$ consists of the cyclic permutation of $(1,4,7)$ together with the transpositions $2 \leftrightarrow 3$ and $5 \leftrightarrow 8$. The index 6 is fixed:

$$\sigma(1) = 4\,,\ \sigma(4) = 7\,,\ \sigma(7) = 1\,,\ \sigma(2) = 3\,,\ \sigma(3) = 2\,,\ \sigma(5) = 8\,,\ \sigma(8) = 5\,,\ \sigma(6) = 6\,.$$

The following theorem establishes the correspondence between conjugacy classes and cycle structures:

Theorem A.3 *Let $\mathrm{id} : X \mapsto X$ be the identity map on $X = \{1, \ldots, s\}$.*

a) For any permutation $\sigma : X \mapsto X$ there exists a permutation $\alpha : X \mapsto X$ and a unique cycle structure C such that $\sigma = \sigma_\alpha^C$.

b) $\sigma_\alpha^C = \alpha \circ \sigma_{\mathrm{id}}^C \circ \alpha^{-1}$ for all permutations $\alpha : X \mapsto X$ and all cycle structures C.

For the proof we refer to the theorems 3.1/3.2 and lemma 3.9 in [12]. Statement a) implies that a unique cycle structure is associated with each permutation. Statement b) implies that any two permutations $\sigma_1 = \sigma_{\alpha_1}^C$ and $\sigma_2 = \sigma_{\alpha_2}^C$ with the same cycle structure C belong to the same conjugacy class represented by the permutation σ_{id}^C. Also, any two representatives σ and $\beta \circ \sigma \circ \beta^{-1}$ of a conjugacy class have the same cycle structure:

$$\sigma = \sigma_\alpha^C = \alpha \circ \sigma_{\mathrm{id}}^C \circ \alpha^{-1} \quad \Rightarrow \quad \beta \circ \sigma \circ \beta^{-1} = \beta \circ \alpha \circ \sigma_{\mathrm{id}}^C \circ \alpha^{-1} \beta^{-1} = \sigma_{\beta \circ \alpha}^C\ .$$

One concludes that the conjugacy classes of permutations on X are in one-to-one correspondence with the cycle structures on X via the natural representative σ_{id}^C.

Result Verification

We have verified the results presented here in both MATHEMATICA version 2.2 and version 3.0. In MATHEMATICA version 2.2 the equivalent of MAPLE's `simplify` with side relations for polynomials can be accomplished by first setting up side relations using Gröbner bases via `AlgebraicRules` and then using some canonical simplification, such as `Factor`, to reduce the order equations modulo the side relations. Note that in

MATHEMATICA version 3.0 `AlgebraicRules` has been superseded by `PolynomialReduce`. Reduction using Gröbner bases can be invoked explicitly using `GroebnerBasis` or implicitly using `Solve`.

A package for deriving order conditions for Runge-Kutta methods, `Butcher.m`, is distributed with MATHEMATICA version 3.0 and is outlined in [15]. Further details are given in the usage notes [10]. A version of the package distributed with version 2.2 also exists, but this is much more limited in scope. We have also implemented our symplectic Runge-Kutta formalism in a public domain MATHEMATICA package, `SymplecticRungeKutta.m`. This package builds upon the functionality provided by `Butcher.m`.