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Explicit Runge–Kutta Pairs with Lower Stage-Order *

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Dedicated to John C. Butcher in
celebration of his eightieth birthday

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Abstract Explicit Runge–Kutta *pairs* of methods of successive orders of accuracy provide effective algorithms for approximating solutions to nonstiff initial value problems. For each explicit RK *method* of order of accuracy p, there is a minimum number s_p of derivative evaluations required for each step propagating the numerical solution. For $p \leq 8$, Butcher has established exact values of s_p, and for $p > 8$, his work establishes lower bounds; otherwise, upper bounds are established by various published methods. Recently, Khashin has derived some new methods *numerically*, and shown that the known upper bound on s_9 for methods of order $p = 9$ can be reduced from 15 to 13. His results motivate this attempt to identify parametrically *exact representations* for coefficients of such *methods*. New *pairs* of methods of orders 5,6 and 6,7 are characterized in terms of several arbitrary parameters. This approach, modified from an earlier one, increases the known spectrum of types of RK *pairs* and their derivations, may lead to the derivation of new RK pairs of higher-order, and possibly to other types of explicit algorithms within the class of general linear methods.

Keywords Runge–Kutta pairs · Order conditions · local error estimation · stage-order

Mathematics Subject Classification (2000) 65L05 · 65L06 · 65L20

1 Introduction

For well-behaved nonstiff vector initial value differential equations

$$y' = f(t, y), \qquad y(t_0) = y_0, \tag{1}$$

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pairs of explicit Runge–Kutta methods are often implemented with adaptive stepsizes to obtain accurate approximations efficiently. With coefficients $a_{i,j}$, c_i selected to yield approximate internal derivative evaluations

$$f_{ni} = f(t_n + c_i h, y_n + h\sum_{j=1}^{i-1} a_{ij} f_{nj}), \qquad i = 1, \ldots, s. \tag{2}$$

two sets of weights b_i, $\widehat{b}_i$ yield endpoint approximations

$$\begin{aligned} y_{n+1} &= y_n + h\sum_{i=1}^{s} b_i f_{ni}, \\ \widehat{y}_{n+1} &= y_n + h\sum_{i=1}^{s} \widehat{b}_i f_{ni}, \end{aligned} \qquad n = 0, 1, \ldots \tag{3}$$

of different orders of accuracy, p and $\widehat{p}$ respectively.[1] Coefficients $\{b_i, a_{i,j}, c_i\}$ are constrained to achieve order p and stability for propagated values, y_{n+1}. For efficiency in computation, attempts are made to find these coefficients so that only a minimum number $s = s_p$ of derivatives is required (see [4, 7]). Weights $\widehat{b}_i$ are selected to give a *matched* method of order $\widehat{p}$ for adaptive stepsize implementation. For $p \le 9$, parametric families of RK pairs of orders $(p, p-1)$ are known requiring $s \ge s_p + 1$ stages, but the results are incomplete.

To facilitate a direct solution of the algebraic order conditions, it is convenient to denote each pair in a Butcher tableau using an $s \times s$ strictly lower-triangular matrix **A**, and s-vectors **b**, $\widehat{\mathbf{b}}$ and $\mathbf{c} = \mathbf{A}\mathbf{e}$ where **e** is the s-vector $[1, .., 1]^t$. (Further, let **C** denote an $s \times s$ diagonal matrix for which $\mathbf{c} = \mathbf{C}\mathbf{e}$.)

Table 1 A Butcher tableau

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^t \\ & \widehat{\mathbf{b}}^t \end{array} \equiv \begin{array}{c|cccc} c_1 & & & & \\ c_2 & a_{21} & & & \\ \cdot & & \cdot\cdot & & \\ c_s & a_{s1} & \cdot\cdot & a_{s,s-1} & \\ \hline 1 & b_1 & & \cdots & b_s \\ 1 & \widehat{b}_1 & & \cdots & \widehat{b}_s \end{array}$$

In this article, new parametric families of RK pairs are derived by directly solving *modified* order conditions expressed using homogeneous polynomials in $a_{i,j}$ and c_i that define *stage-order*.

DEFINITION 1

Let p_i denote the stage-order of stage i if *subquadrature* equations defined by

$$q_i^k \equiv \sum_{j=1}^{i-1} a_{ij} c_j^{k-1} - \frac{c_i^k}{k} = 0, \qquad k = 1, .., p_i, \quad i = 1., , .s, \tag{4}$$

[1] Usually $\widehat{p} = p - 1$, as for pairs derived here. For examples of other types, see [10, 19].

and *stage-dissociation* constraints

$$\sum_{c_k=c_j} a_{ik} = 0, \qquad p_i > p_j + 1, \tag{4'}$$

are satisfied. Also, the first (approximating) formula in (3) is said to have stage-order p if the *quadrature* conditions

$$\sum_{j=1}^{i-1} b_i c_i^{k-1} - \frac{1}{k} = 0, \qquad k = 1, .., p, \tag{4''}$$

hold; the second (error-estimating) formula in (3) is said to have stage-order $\tilde{p}$ if these conditions hold for weights $\widehat{b}_i$ when p is replaced by $\tilde{p}$. (It is possible that $\tilde{p} = p > \widehat{p}$, since formula (3) for $\widehat{y}_{n+1}$ may have order p for quadrature problems; see Tables 4 and 5 as illustrations.)

If (3) have stage-orders $p, \tilde{p},\ p \geq \tilde{p} \geq \widehat{p}$, we distinguish each type of RK pair by its *augmented* stage-order vector $ASOV = (p_1, .., p_s : p, \tilde{p})$. ASOV vectors for several known pairs appearing in [22,23], and as well for new pairs derived below, are appended (as columns) to corresponding Butcher tableaux. A related distinguishing feature of each family is its *dominant stage-order*

$$\text{DSO} = \min_i \big\{\ p_i \mid \sum_{c_j=c_i} b_j \neq 0, \quad i = 1, \ldots, s\big\}. \tag{5}$$

(Usually, when at least p nodes are distinct and corresponding weights are nonzero, the DSO is determined by nonzero weights, b_i.)

Motivated by techniques for deriving *methods* in [3,9] and *pairs* in [12], the author has developed several strategies for solving the order conditions directly. These led to parametric families of effective RK *pairs* [18–21,23,24], with $p = 6, .., 9$ and DSO=p-4. When $p = 6, 7,\ s = s_p + 1$ where s_p is minimal for the higher-order method of each pair. When $p = 8, 9$ or otherwise for some pairs with DSO=p-3 in [17], the required number of stages is slightly larger than $s_p + 1$. Yet since 1978, there has been no reduction in the total numbers of stages required for such *pairs*. In contrast, searches for high-order *methods* have provided sharper upper bounds to $s_p,\ p > 9$ [11,13,16].

Recently, numerical iterative solutions to the order equations developed by Khashin[14] have provided new *methods* with DSO<p-4,[2] albeit, when $p = 6, 7, 8$, requiring only the known minimum number $s = s_p$ of stage evaluations. Moreover, for $p = 9$, he has found methods requiring only $s = 13$ stages, a remarkable advance on the previous $s = 15$ stages required in the methods of order 9 in each pair of [18,19]. (Butcher[5] has shown that $s_9 \geq 12$.)

As observed in [23], "the characterization of various *types* of methods of orders $p > 5$ remains incomplete" (see also [8,15]). In [23,24], confining the

[2] The Hairer 17-stage method [13] of order 10 with DSO=5 requires a quadrature rule with Gaussian nodes, thereby making a reliable error estimator of order $p - 1$ difficult without several additional stages at least. Tables 4,5 below illustrate this hazard.

dimensions of certain subspaces $\boldsymbol{\Lambda}_r$, $\boldsymbol{\Theta}_r$ (defined below), and imposing constraints on the coefficients to force pairwise annihilation of these subspaces led to the characterization of new pairs with DSO=p-4 (with all nodes distinct).

In the development in [14], subspaces related to $\boldsymbol{\Theta}_r$ lead to additional equations used in the numerical solution of the order equations. Here, the approach in [23] is adapted to find exact formulas for coefficients of some families of these new *methods*, and thereafter to derive parametric families of new *pairs* of RK methods with stage-orders *lower* than those for currently well-known families.

The next section reviews the modified order conditions. Section 3 surveys tools used to solve the order conditions directly. Sections 4 and 5 report new families of pairs, and provides examples illustrating features that differentiate them from known formulas. Section 6 motivates continuing research.

2 The order conditions and other notation

In [2,6], Butcher tabulates standard order conditions for a method of order p as an isomorphism from functions on *rooted trees*. Equivalent *modified* order conditions developed in [17,23,24] are used here, and assume a knowledge of the theory based on rooted trees. For the tree τ with one node of height $H(\tau) = 0$, trees $t = [t_1, \ldots, t_k]$ are defined recursively: for t_i having r_i nodes and height $H(t_i)$, t is the tree of $1+r_1+\ldots+r_k$ nodes and height $1+\max_i\{H(t_i)\}$ obtained by grafting the k trees to a single additional node called the root. For example, each *bushy* tree $[\tau, \ldots, \tau] \equiv [\tau^k]$ is the tree with k nodes attached to a root, and height $H(t) = 1$; the *tall* tree $t = [[[\tau]]]$ has four nodes and height $H(t) = 3$.

For each tree of height $H(t) \geq 2$, and the associated standard order condition, there corresponds a *modified* order condition expressed in terms of *subquadrature* s-vectors

$$\mathbf{q}^{[k]} \equiv \mathbf{A}\mathbf{C}^{k-1}\mathbf{e} - \frac{1}{k}\mathbf{C}^k\mathbf{e}, \quad k = 1, \ldots, p-2, \tag{4'''}$$

with components of $\mathbf{q}^{[k]}$ given by (4). With the slight notational differences, $\mathbf{B} := \mathbf{A}$, $\mathbf{D} := \mathbf{C}$, $a_i := c_i$, $c_k := \mathbf{q}^{[k]}$, these modified forms (see (4.20)* and the Appendix in [1]) of the standard order conditions were previously derived by Albrecht while obtaining matrix forms of the standard Runge–Kutta methods through extending A-B methods formulated by Butcher in [3]. Albrecht's approach provides a detailed proof of the equivalence of the two forms of order conditions. In contrast, the *structure* of these modified order conditions is exploited here for *deriving* new methods and pairs of methods. To represent *modified* order conditions, we need premultiplication of $\mathbf{q}^{[k]}$ by each of $\mathbf{A}$ and $\mathbf{C}$, and component-wise products of such expressions.

DEFINITION 2

For $\rho^{[k,k]} = \mathbf{q}^{[k]}$, recursively define for increasing algebraic degree $r > k \geq 2$, and each vector of positive integers $[l_1, \ldots, l_m]$, vectors of the form:

$$\rho^{[r,k]} = \mathbf{AC}^{l_1-1} \ldots \mathbf{AC}^{l_m-1}\mathbf{q}^{[k]}, \tag{6}$$
$$m > 0, \quad 3 \leq r = l_1 + \ldots + l_m + k < p.$$

DEFINITION 3

For $\mathbf{R}^{[r,k,0]} = \rho^{[r,k]}$, $r \geq k \geq 2$, recursively define for an increasing number n of side branches of height $H(t_i) \geq 1$, matrix products by $\mathbf{A}$ and $\mathbf{C}$ of *component-wise* product (denoted *) vectors of the form:

$$\mathbf{R}^{[r,k,n]} = \mathbf{AC}^{l_1-1} \ldots \mathbf{AC}^{l_m-1}\left(\mathbf{R}^{[r_1,k_1,n_1]} * \mathbf{R}^{[r_2,k_2,n_2]}\right), \tag{7}$$

$$m \geq 0, \quad n = n_1 + n_2 + 1, \quad k = k_1 + k_2, \quad 4 \leq r = l_1 + \ldots + l_m + r_1 + r_2 < p.$$

These recursive definitions are conveniently sequenced by any total ordering of all rooted trees up to p nodes. These are used in refining the partition of the modified order conditions identified in [24] wherein the numbers of each type of partitioned order conditions are given for methods up to order 10.

THEOREM 1

A method defined by $\{\mathbf{b}^t, \mathbf{A}, \mathbf{C}\}$ is of order p if and only if the coefficients satisfy the following order conditions.

I. **The quadrature conditions** which correspond precisely to the bushy trees τ and $[\tau^{k-1}]$ (having $k-1$ nodes attached to the root):

$$\mathbf{b}^t\mathbf{C}^{k-1}\mathbf{e} = \frac{1}{k}, \qquad k = 1, \ldots, p; \tag{8}$$

II. **The subquadrature conditions** which correspond precisely to the tall trees of heights $H(t)$, $2 \leq H(t) < p$ (with no *side* branches):

$$\mathbf{b}^t\mathbf{A}^{m-1}\mathbf{q}^{[k]} = 0, \qquad m \geq 1, \quad k \geq 2, \quad 3 \leq m + k \leq p; \tag{8$'$}$$

III. **The extended subquadrature conditions** which correspond to trees having one or more side branches with $l_i > 1$ and height $H(t_i) = 0$ for some $i: \ 0 \leq i \leq m$:

$$\mathbf{b}^t\mathbf{C}^{l_0-1}\rho^{[r,k]} = 0, \qquad l_0 \geq 1, \quad , r \geq k \geq 2, \quad 4 \leq l_0 + r \leq p; \tag{8$''$}$$

IV. **The nonlinear order conditions** corresponding to trees that have at least one *side* branch with height $H(t_i) \geq 1$ grafted to the highest stem:

$$\mathbf{b}^t\mathbf{C}^{l_0-1}\mathbf{R}^{[r,k,n]} = 0, \qquad n > 0, \ l_0 \geq 1, \ r \geq k \geq 4, \ l_0 + r \leq p. \tag{8$'''$}$$

Proof :

These four categories partition the order conditions tabulated in [6] by identification to all possible rooted trees with no more than p nodes. Each of the conditions above is either a quadrature order condition (8) (corresponding to rooted trees of height $H(t) = 0$ or 1), or else one of the *annihilating* order conditions of the form

$$\mathbf{b}^t \boldsymbol{\Psi}(t) = 0, \qquad \text{for each tree } t \text{ with } H(t) \geq 1, \tag{9}$$

shown *recursively* in [23,24] to be equivalent to a linear combination of the standard order conditions $\Phi(t) \equiv \mathbf{b}^t \phi(t) = \frac{1}{\gamma(t)}$ in [6].[3] In (9), the vector $\boldsymbol{\Psi}(t)$ is the *compound* weight function obtained precisely by replacing each occurrence of $\mathbf{A}\mathbf{C}^{k-1}\mathbf{e}$ within $\phi(t)$ of the standard order condition by $\mathbf{q}^{[k]}$.

The quadrature conditions (8) are common to both the standard set of quadrature conditions, and the modified conditions stated both in [24] and above. For each tall tree, the modified order condition (8′) gives

$$\mathbf{b}^t \mathbf{A}^{r-1} \mathbf{q}^{[k]} \equiv \mathbf{b}^t \mathbf{A}^r \mathbf{C}^{k-1} \mathbf{e} - \mathbf{b}^t \mathbf{A}^{r-1} \frac{\mathbf{C}^k \mathbf{e}}{k} = 0$$

since the standard order condition for a tall tree yields $\mathbf{b}^t \mathbf{A}^{r-1} \mathbf{C}^k \mathbf{e} = \frac{k!}{(k+r)!}$. Such a linear combination of *standard* subquadrature (and when $r = 1$ quadrature) conditions sequentially implies the equivalence to a corresponding *modified* subquadrature condition. The equivalence of each *modified* extended subquadrature condition (8″) terminating in a single vector $\mathbf{q}^{[k]}$ to a linear combination of corresponding *standard* order conditions defined by products of powers of matrices $\mathbf{A}$ and $\mathbf{C}$ with $\mathbf{C}^k\mathbf{e}$ and $\gamma(t)$ is similar: again there are only two terms in the expansion of the former, and in this case the same factors, $(k + \tilde{r})$ say, in the denominators of each as well as for the $\gamma(t)$ terms in the standard order conditions are omitted for each internal occurrence of $\mathbf{C}$ for both types. Each *modified* non-linear quadrature condition (8‴) contains multiplicative factors $\mathbf{R}^{[r,k,0]} = A..\mathbf{q}^{[k]}$ each of which has two terms on expansion of $\mathbf{q}^{[k]}$. For n side branches of height $H(t_i) \geq 1$, there will be a total of 2^{n+1} terms in a full expansion: when these are replaced by expressions of $\frac{1}{\gamma(t_j)}$ from the *standard* order conditions, the linear combination will have a value of zero to show that the modified non-linear condition is just a linear combination of standard order conditions, at least one of which will be non-linear. As this equivalence is developed recursively beginning with the quadrature conditions common to both, equivalence of these modified versions to the standard order conditions is established. (There is some duplication within the modified forms which is utilized later in solving the order conditions.)

Yet another proof of the equivalence of these two sets of order conditions in implicit in the development by Albrecht [1]. □

In contrast to the derivation of matrix formulated order conditions in [1], the present approach focuses on partitioning the modified order conditions by four different types to facilitate their direct solution.

[3] $\phi(t)$ denotes the vector $[\Phi_1(t), ..., [\Phi(t)_s]$ defined by Butcher [6] (see Lemma 312B).

3 Devices for solving the order conditions

The difficult challenge has been solution of the order conditions for over a century. Here, the phases of solution expounded in [23] are adapted to deriving *methods* and *pairs of methods* of lower stage-order. The motivation for constructing methods of lower stage-order is mainly to determine whether such methods can yield more efficient algorithms than those already known. The results obtained by Khashin [14] show that the minimum number of stages for a method of order 9 has been reduced from the previously known lower limit of 15 in [18,19] to 13. Should *pairs* of methods with a reduction in the number of stages be possible, this may lead to more efficient algorithms.

3.1 Annihilating homogeneous polynomials

Orthogonality of $\mathbf{b}^t$ to many vectors of $\mathbb{R}^s/\mathbf{e}_1$, (the set of vectors in $\mathbb{R}^s$ with first element equal to zero), is basic to the derivation of new RK formulas. Since $\mathbf{b}^t\mathbf{e} = 1$, the nullspace of $\mathbf{b}^t$ has dimension $s-1$. Further, for nontrivial methods with $p \geq 2$, $(I - 2\mathbf{C})\mathbf{e}$ is in this nullspace, but not in $\mathbb{R}^s/\mathbf{e}_1$.

As each vector multiplying $\mathbf{b}^t$ on the right of $(8')$, $(8'')$, $(8''')$ is a matrix or component-wise product with one or more factors $\mathbf{q}^{[k]}$, it lies in $\mathbb{R}^s/\mathbf{e}_1$, and is orthogonal to $\mathbf{b}^t$. Since the total number of conditions in this set is $N_p - s$, one for each order condition other than the quadrature conditions (8), it follows that these $N_p - s$ vectors lie in a subspace of dimension $s-2$ of the nullspace of $\mathbf{b}^t$. Furthermore, this sub-nullspace also contains all of the remaining combinations of the form $\{[kC^{k-1} - (k+1)C^k]\mathbf{e},\ k = 2, .., p-1\}$ determined from the quadrature order conditions (8).[4]

The essence of the construction of new methods is to select a basis of $s-2$ of these $N_p - 2$ vectors in $\mathbb{R}^s/\mathbf{e}_1$, and then impose constraints which force each of those remaining to lie in their span. The selection is developed by refining similar orthogonal properties from [23] through left and right subspaces of increasing homogeneous degree. Each new subspace is defined as the span of pre- or post-multiplication of the vectors in the subspaces containing vectors of the next lower homogeneous degree, together with component-wise products of two or more homogeneous polynomials of lower degree. For example, $\mathbf{A}\boldsymbol{\Theta}_{r-1}$ specifies pre-multiplication of each (column) vector of $\boldsymbol{\Theta}_{r-1}$ by the matrix $\mathbf{A}$, and $\boldsymbol{\Lambda}_{r-1}\mathbf{A}$ specifies the post-multiplication of each (row) vector of $\boldsymbol{\Lambda}_{r-1}$ by the same matrix; as well, $\boldsymbol{\Theta}_4$ contains ${\mathbf{q}^{[2]}}^2$, for example. This recursive definition of the appropriate subspaces emphasizes the uniformity of the underlying linear algebraic structure within the order equations. In turn, this motivates the approach to solving the order conditions, and perhaps may assist in ways to determine exact constraints on the arbitrary nodes (and other parameters) which remain.

[4] To illustrate, the 8 order conditions of order 4 imply that the nullspace of $\mathbf{b}^t$ contains the subspace of dimension 2, $\left\langle \mathbf{q}^{[2]}, \mathbf{C}\mathbf{q}^{[2]}, \mathbf{A}\mathbf{q}^{[2]}, \mathbf{q}^{[3]}, (2\mathbf{C} - 3\mathbf{C}^2)\mathbf{e}, (3\mathbf{C}^2 - 4\mathbf{C}^3)\mathbf{e} \right\rangle \in \mathbf{R}^s/\mathbf{e}_1$, and as well $(I - 2\mathbf{C})\mathbf{e}$.

DEFINITION 4

Let **right homogeneous subspaces** be defined recursively to be the spanning sets of those vectors of increasing degree $r \geq 2$ lying within

$$\boldsymbol{\Theta}_2 = \left\langle \mathbf{q}^{[2]} \right\rangle, \tag{10}$$

$$\boldsymbol{\Theta}_r = \left\langle \mathbf{q}^{[r]}, \mathbf{A}\boldsymbol{\Theta}_{r-1}, \mathbf{C}\boldsymbol{\Theta}_{r-1}, \boldsymbol{\Theta}'_r \right\rangle, \qquad 3 \leq r < p, \tag{10$'$}$$

where

$$\boldsymbol{\Theta}'_r = \left\langle \mathbf{R}^{[r,k,n]}, \quad n > 0,\ r \geq 4 \right\rangle. \tag{10$''$}$$

Each $\boldsymbol{\Theta}_r$ is a subspace of $\mathbb{R}^s/\mathbf{e}_1$, and is isomorphic to the subspace obtained from L'_r defined by Khashin [14] when the last component of L'_r is removed. (Some care is needed in denoting vectors of $\boldsymbol{\Theta}_r$ lying in these subspaces. In [14], vectors of L'_3 should contain only polynomials of homogeneous degree 3: some vectors that are reported therein to lie within L'_3, and as well, the vector $(\tilde{A}^2\mathbf{e} - \tilde{A}\mathbf{e} * \tilde{A}\mathbf{e}/2)^2$ actually lie in L'_4.) To illustrate, we observe that $\boldsymbol{\Theta}_1$ is empty, $\boldsymbol{\Theta}_2 =< \mathbf{q}^{[2]} >$, $\boldsymbol{\Theta}_3 =< \mathbf{q}^{[3]}, \mathbf{A}\mathbf{q}^{[2]}, \mathbf{C}\mathbf{q}^{[2]} >$, while $\boldsymbol{\Theta}_4$ contains analogous vectors, and also ${\mathbf{q}^{[2]}}^2$.

DEFINITION 5

Let **left homogeneous subspaces** be defined recursively to be the spanning sets of those vectors of increasing degree $r \geq 1$ lying within

$$\boldsymbol{\Lambda}_1 = \left\langle \mathbf{b}^t \right\rangle, \tag{11}$$

$$\boldsymbol{\Lambda}_r = \left\langle \boldsymbol{\Lambda}_{r-1}\mathbf{A}, \boldsymbol{\Lambda}_{r-1}\mathbf{C}, \mathbf{b}^t * \boldsymbol{\Theta}_{r-1} \right\rangle, \qquad 2 \leq r < p-1. \tag{11$'$}$$

In particular, $\boldsymbol{\Lambda}_1 =< \mathbf{b}^t >, \boldsymbol{\Lambda}_2 =< \mathbf{b}^t\mathbf{A}, \mathbf{b}^t\mathbf{C} >,\ \boldsymbol{\Lambda}_3 =< \mathbf{b}^t\mathbf{A}^2, \mathbf{b}^t\mathbf{AC}, \mathbf{b}^t\mathbf{CA}, \mathbf{b}^t\mathbf{C}^2, \mathbf{b}^t * \mathbf{q}^{[2]} >$. (Observe that $\boldsymbol{\Lambda}_3$ contains both the vector-matrix product, $\mathbf{b}^t(\mathbf{AC} - \mathbf{C}^2/2)$, and the component-wise product of two vectors, $\mathbf{b}^t * \mathbf{q}^{[2]}$, that *appear* the same, but are generically different vectors.)

THEOREM 2

Suppose for given p and s, the weights b_i and nodes c_i of a method are selected to satisfy the quadrature order conditions (8). The method is of order p, if in addition the left homogeneous polynomials *annihilate* the right homogeneous polynomials so that for $L_{r_1} \in \boldsymbol{\Lambda}_{r_1},\ R_{r_2} \in \boldsymbol{\Theta}_{r_2}$,

$$L_{r_1} \cdot R_{r_2} = 0, \quad \text{whenever} \ \ 2 < r_1 + r_2 \leq p. \tag{12}$$

Proof :

This is a restatement of Theorem 1 using the quadrature conditions, and the left and right homogenous polynomials. The duplication in (12) is intentional: it facilitates constraints on dimensions of both left and right subspaces and allows linear dependencies among vectors they contain. (Again, the quadrature conditions may be replaced by $\mathbf{b}^t\mathbf{e} = 1$, and the orthogonality of $\mathbf{b}^t$ to certain polynomials in $\mathbf{C}^k\mathbf{e}$. See also Definition 7 later.) □

For all known methods and pairs, order conditions of type (8‴) were satisfied because certain individual components of either left or right homogeneous polynomials, lying in $\boldsymbol{\Lambda}_r$, $\boldsymbol{\Theta}_r$ respectively, were equal to zero. In contrast, for lower stage-order methods and pairs derived here, these order conditions are satisfied by less-restrictive (linear dependence) constraints.

3.2 Selecting augmented stage-order vectors

In previous work, [18, 20, 23] stage-order vectors were specifically selected so that either $DSO = p - 4$ or $DSO = p - 3$. For new methods and pairs, the dominant stage-orders are lower but not a linear function of the order; rather, we utilize the stage-order vectors which can be identified from methods displayed by Khashin [14]. Selected ASOV vectors are tabulated with the numbers of arbitrary parameters for several families in Table 2.

Table 2 Augmented Stage-order Vectors and Arbitrary Parameters (AP) for New Formulas

Type	s	p	DSO	AP	ASOV	Comment
[14](4.1,Eg.1)	7	6	1	3	(6,1,1,1,1,1,3:6)	Exact
New pair	8	6,5	1	3+2	(6,1,1,1,1,1,3,1:6,5)	Exact, Reliable
[14](4.1,Eg.2)	7	6	2	3	(6,1,2,2,2,1,2:6)	Exact
New pair	8	6,5	2	3+3	(6,1,2,2,2,1,2,2:6,6)	Exact, Unreliable
[14](4.2,Eg.2,3)	9	7	2	6	(7,1,2,2,2,2,2,2,2:7)	Inexact
New pair	10	7,6	2	6+3	(7,1,2,2,2,2,2,2,2,2:7,6)	Inexact, Reliable

3.3 Satisfying the subquadrature conditions

For at least p distinct nodes, the quadrature conditions are usually satisfied by selecting the remaining $s-p$ nodes and corresponding weights arbitrarily, and using a van der Monde matrix based on the distinct nodes to specify p weights directly. In some *singular* methods, the determined weights can be satisfied using fewer distinct nodes which satisfy certain orthogonality conditions. Examples of some singular formulas appear in [13–15, 22] and in Tables 4 and 5 below.

On requiring the particular left homogeneous polynomial row vectors

$$\mathbf{B}^{[r]} = \mathbf{b}^t\mathbf{A}^r, \qquad r = 0, \ldots, 3, \tag{13}$$

to satisfy

$$\sum_{i=1}^{s} B_i^{[r]} c_i^{k-1} \equiv \mathbf{b}^t\mathbf{A}^r\mathbf{C}^{k-1}\mathbf{e} = \frac{(k-1)!}{(k+r)!} \qquad k = 1, \ldots, p-r-1, \tag{14}$$

most of the subquadrature conditions (8′) are satisfied. Those (with $r > 3$) remaining will be satisfied by linear dependencies within subspaces $\boldsymbol{\Lambda}_r$.

With $\mathbf{B}^{[1]} \equiv \mathbf{b}^t\mathbf{A} = \mathbf{b}^t(\mathbf{I} - \mathbf{C})$, and additional constraints on $\mathbf{B}^{[2]}, \mathbf{B}^{[3]}$, extended order conditions of (8″) requiring $\mathbf{b}^t\mathbf{C}^l\mathbf{A}^{r-1}\mathbf{q}^{[k]} = 0,\ 2 < k+r+l \leq p$ are satisfied.

Table 3 Triangular tableau of homogeneous polynomials

$$\begin{array}{c|cccc} c_1 & & & & \\ c_2 & B_1^{[s-1]} & & & \\ . & . & .. & & \\ c_s & B_1^{[1]} & .. & B_{s-1}^{[1]} & \\ \hline 1 & B_1^{[0]} & & \cdots & B_s^{[0]} \end{array} \equiv \begin{array}{c|cccc} c_1 & & & & \\ c_2 & b_s a_{s,s-1}..a_{21} & & & \\ . & . & .. & & \\ c_s & \sum b_{i_0} a_{i_0 1} & .. & b_s a_{s,s-1} & \\ \hline 1 & b_1 & & \cdots & b_s. \end{array}$$

Values of all homogeneous polynomials (13) form an array isomorphic to a Butcher tableau of coefficients. If the diagonal elements of Table 3 are non-zero, the coefficients of a method are uniquely determined by the back-substitution (used in [18]):

$$a_{k,k-l} = \frac{B_{k-l}^{[s-k+1]} - \sum_{i=k-l+1}^{k-1} B_i^{[s-k]} a_{i,k-l}}{B_k^{[s-k]}}, k = s, .., 1, l = 1, .., k-1. \quad (15)$$

For example, for $k = s-1,\ l = 3,\ k-l = s-4$,

$$a_{s-1,s-4} = \left[\left(\sum_{i>j=s-3}^{s} b_i a_{i,j} a_{j,s-4} \right) - \sum_{j=s-3}^{s-2} \left(\sum_{i=j+1}^{s} b_i a_{i,j} \right) a_{j,s-4} \right] / b_s a_{s,s-1}.$$

In practice, $\{a_{i,j},\ i \le s-3\}$ will be computed using using the subquadrature equations (4) and linear dependencies specified for each family, and (15) will be utilized only for larger values of $i \ge s-2$.

It turns out that the quadrature conditions (8) together with (14) for all $r < p$ are precisely the order conditions required for a method to be of order p for systems of linear constant coefficient differential equations. In deriving parametric families that follow, we show how to select these homogeneous polynomials so that conditions (14) are valid.

3.4 Imposing Linear Dependence to satisfy remaining Order Conditions

DEFINITION 6
Define direct sums of left and right annihilating subspaces by

$$\mathcal{L}_r = \left\langle \cup_{k=1}^{r} \boldsymbol{\Lambda}_k \right\rangle \quad r = 1, \ldots, p-1, \quad (16)$$
$$\mathcal{R}_r = \left\langle \cup_{k=2}^{r} \boldsymbol{\Theta}_k \right\rangle, \quad r = 2, \ldots, p-1. \quad (17)$$

In [14], $\mathbf{M}'_r$ (with the final component omitted) denotes $\mathcal{R}_r$, and Khashin explores the dimensions of $\mathbf{M}'_r$ and of $\mathbf{B}'_r = \mathbf{M}'_r/\mathbf{M}'_{r-1}$ in analyzing new types of methods with $s = s_p$. More is possible: the dimensions of $\mathcal{L}_{p-r}$ complement the dimensions of $\mathcal{R}_r$ by Theorem 2. As well, [23,24] use orthogonality of $\mathbf{b}^t,\ \mathbf{b}^t\mathbf{C},\ \mathbf{b}^t\mathbf{C}^2$ to polynomials defined by

DEFINITION 7

$$\omega_r(c) = \frac{d^2}{dc^2}[c^r(1-c)^2], \quad r = 2, .., p-2, \tag{18}$$

and

$$\overline{\omega}_r(c) = \frac{d^3}{dc^3}[c^r(1-c)^3] \equiv r\omega_{r-1}(c) - (r+3)\omega_r, \quad r = 3, .., p-2, \tag{19}$$

to construct some families of RK pairs with DSO=p-4. Since $\overline{\omega}_r(0) = 0,\ r > 3$, and $\overline{\omega}_4(\mathbf{C})\mathbf{e}$ must be orthogonal to each vector generating $\boldsymbol{\Lambda}_r,\ r = 1, 2, 3$ defined by $(11')$, we may assume for $p = 7$ without loss of generality that $\overline{\omega}_4(\mathbf{C})\mathbf{e} \in \mathcal{R}_4$. Such assumptions for other values of p are possible [24].

To illustrate what might be possible, *suppose* $\{\mathbf{q}^{[2]},\ \mathbf{C}\mathbf{q}^{[2]}\}$ forms a basis of $\mathcal{R}_3$. Then constants F_i, G_i exist with

$$\mathbf{A}\mathbf{q}^{[2]} = (F_1 + F_2\mathbf{C})\mathbf{q}^{[2]}, \tag{20}$$

$$\mathbf{q}^{[3]} = (G_1 + G_2\mathbf{C})\mathbf{q}^{[2]}. \tag{21}$$

Additional linear dependence in $\langle \mathcal{R}_4,\ \overline{\omega}_4(\mathbf{C})\mathbf{e} \rangle$ occurs if H_i, J_i, K_i exist with

$$\mathbf{A}\mathbf{C}\mathbf{q}^{[2]} = (H_1 + H_2\mathbf{C} + H_3\mathbf{C}^2)\mathbf{q}^{[2]} + H_4\overline{\omega}_4(\mathbf{C})\mathbf{e} \tag{22}$$

$$\mathbf{q}^{[4]} = (J_1 + J_2\mathbf{C} + J_3\mathbf{C}^2)\mathbf{q}^{[2]} + J_4\overline{\omega}_4(\mathbf{C})\mathbf{e} \tag{23}$$

$$(\mathbf{q}^{[2]})^2 = (K_1 + K_2\mathbf{C} + K_3\mathbf{C}^2)\mathbf{q}^{[2]} + K_4\overline{\omega}_4(\mathbf{C})\mathbf{e} \tag{24}$$

Other choices appear in [23]. Pre-multiplication of formal vectors of $\mathcal{R}_3$ by powers of $\mathbf{A}$ and $\mathbf{C}$ yield the remaining formal vectors of $\mathcal{R}_4$: those for (20) are

$$\mathbf{A}^2\mathbf{q}^{[2]} = (F_1\mathbf{A} + F_2\mathbf{A}\mathbf{C})\mathbf{q}^{[2]} \tag{20'}$$

$$\mathbf{C}\mathbf{A}\mathbf{q}^{[2]} = (F_1 + F_2\mathbf{C})\mathbf{C}\mathbf{q}^{[2]} \tag{20''}$$

In consequence, each left homogeneous polynomial orthogonal to the basis $\{\mathbf{q}^{[2]},\ \mathbf{C}\mathbf{q}^{[2]},\ \mathbf{C}^2\mathbf{q}^{[2]},\ \overline{\omega}_4(\mathbf{C})\mathbf{e}\}$, of $\mathcal{R}_4$, is also orthogonal to all vectors of $\mathcal{R}_4$.

Conversely, constraints imposed on the homogeneous polynomials specified by (14) imply $\mathbf{b}^t$ is orthogonal to $\mathbf{A}^r\mathbf{q}^{[k]}$ for $r \geq 0,\ k \geq 2,\ 2 \leq r + k < p$, and through the linear combinations, these imply orthogonality to other right homogeneous polynomials. This particular choice of basis for $\mathcal{R}_4$ motivates those selected below for each family of order $p = 6$ or $p = 7$ considered. Conditions necessary and sufficient for a formula to be of order p are motivated, and formal algorithms for computation of all coefficients for both methods and pairs are expressed as functions of their arbitrary parameters.

4 Parametric formulation of Runge–Kutta pairs of orders 6 and 5

Here, the tools surveyed in Section 3 are applied, with elaboration as appropriate, to construct algorithms for computing coefficients of methods and pairs as functions of user-selected parameters.

4.1 Unreliable Runge–Kutta pairs

We begin with an algorithm for a three-parameter family of methods of order 6 based on the method of Example 4.2 in Section 4.1 in [14]. The example in Table 4 illustrates the general structure of Runge–Kutta *pairs* based on methods of this type.

Table 4 RK(8-6:5)a: an unreliable 8-stage 6,5 pair of type Khashin [14] 4.1(3)

0									6
$\frac{1}{5}$	$\frac{1}{5}$								1
$\frac{1}{4}$	$\frac{3}{32}$	$\frac{5}{32}$							2
$\frac{4}{7}$	$\frac{60}{343}$	$-\frac{440}{343}$	$\frac{576}{343}$						2
$\frac{7}{9}$	$\frac{847}{17496}$	$\frac{770}{729}$	$-\frac{17024}{19683}$	$\frac{84721}{157464}$					2
$\frac{1}{5}$	$\frac{523}{2240}$	0	$-\frac{5}{57}$	$\frac{245}{2496}$	$-\frac{1215}{27664}$				1
1	$\frac{15}{2212}$	$\frac{314}{395}$	$\frac{3448}{1501}$	$-\frac{2695}{4108}$	$\frac{203391}{273182}$	$-\frac{864}{395}$			2
$\frac{4}{7}$	$\frac{1185}{10976}$	$-\frac{2543}{1715}$	$\frac{36262}{19551}$	$-\frac{245}{1248}$	$\frac{1215}{13832}$	$\frac{1}{5}$	0		2
1	$\frac{43}{560}$	$\frac{1}{5}$	$\frac{2816}{7695}$	$\frac{16807}{84240}$	$\frac{19683}{69160}$	$-\frac{1}{5}$	$\frac{79}{1080}$	0	6
1	$\frac{43}{560}$	$-\frac{1}{5}$	$\frac{2816}{7695}$	$-\frac{41}{84240}$	$\frac{19683}{69160}$	$\frac{1}{5}$	$\frac{79}{1080}$	$\frac{1}{5}$	6

Stages {1,3,4,5,7} of each method in this family have stage-order 2 (or 3 if $c_3 = 3c_2/2$). As well, stages {2,6} have stage-order 1 with $c_2 = c_6$ and $b_2 + b_6 = 0$. The formula for choosing c_4 is precisely that found in [18], and this choice may be motivated with an argument similar to that used therein. The subsequent choice for c_5 is specified so that the five stages with DSO=2 are sufficient to satisfy a quadrature rule of order 6. (For each stage, the stage-order is appended on the right of Table 4.)

For this family, $\mathbf{C}\mathbf{q}^{[2]} \equiv c_2\mathbf{q}^{[2]} = [0, -c_2^3/2, 0, 0, 0, -c_2^3/2, 0]$. Hence, in contrast to (20), we select $\{\mathbf{q}^{[2]},\ \mathbf{q}^{[3]}\}$ as a basis for $\mathcal{R}_3$ and impose the constraint

$$\mathbf{A}\mathbf{q}^{[2]} = F_1\mathbf{q}^{[2]} + F_2\mathbf{q}^{[3]}. \tag{25}$$

ALGORITHM 1.1

A 3-parameter family of 7-stage methods of order 6 with DSO=2:

1. With $c_2,\ c_3$ arbitrary, choose nodes c_1, c_3, c_4, c_5, c_7 distinct and in [0,1], by $$c_1 = 0,\ c_4 = \frac{c_3}{15c_3^2 - 10c_3 + 2},\ c_5 = \frac{\int_0^1 c^2(c-c_3)(c-c_4)(c-c_7)dc}{\int_0^1 c(c-c_3)(c-c_4)(c-c_7)dc},\ c_7 = 1,$$ and $c_6 = c_2$.
2. Compute $a_{2,1} = c_2$.
3. As $q_3^{[1]} = q_3^{[2]} = 0$, compute $a_{3,2} = \dfrac{c_3^2}{2c_2}, \quad a_{3,1} = c_3 - a_{3,2}$.

4. As $q_3^{[2]} = 0$, compute $F_2 = \dfrac{a_{3,2}q_2^{[2]}}{q_3^{[3]}}$. Apply (25) for stage 4 with $q_4^{[1]} = q_4^{[2]} = 0$ to obtain
$$a_{4,2} = \frac{c_4^2(3c_3 - 2c_4)}{2c_2c_3}, \quad a_{4,3} = \frac{c_4^2(c_4 - c_3)}{c_3^2}, \quad a_{4,1} = c_4 - a_{4,2} - a_{4,3}.$$
5. Choose homogeneous polynomials $B_i^{[k]}$ defined in (13) as follows:
   (a) Let b_2 be arbitrary, with $B_6^{[0]} = -B_2^{[0]} \equiv -b_2$. Compute $B_i^{[0]}$, to satisfy
$$\mathbf{B}^{[0]}\mathbf{C}^{k-1}\mathbf{e} = \frac{1}{k}, \quad k = 1, .., 5.$$
   (The choice of c_5 implies this condition is valid for $k = 6$ as well.)
   (b) Choose $B_i^{[1]} = B_i^{[0]}(1 - c_i), \quad i = 1, .., 6.$
   (c) Choose $B_2^{[2]} = 0$, and $B_i^{[2]}$, $i = 1, 3, 4, 5$, to satisfy
$$\mathbf{B}^{[2]}\mathbf{C}^{k-1}\mathbf{e} = \frac{(k-1)!}{(k+2)!}, \quad k = 1, .., 4.$$
   (d) Choose $B_2^{[3]} = 0$, and $B_i^{[3]}$, $i = 1, 3, 4$, to satisfy
$$\mathbf{B}^{[3]}\mathbf{C}^{k-1}\mathbf{e} = \frac{(k-1)!}{(k+3)!}, \quad k = 1, .., 3.$$
6. Observe that $\{b_i = B_i^{[0]}, \ i = 1, .., 7\}$, and apply the back-substitution algorithm (15) to $\{\mathbf{B}^{[k]}, \ k = 1, 2, 3, \}$ to compute the remaining coefficients $\{a_{i,j}, \ i = 5, 6, 7\}$.

ALGORITHM 1.2

A 6-parameter family of 8-stage 6,5 RK pairs with DSO=2: after choosing the first seven stages $\{b_i, a_{i,j}, c_i, \ 1 \le i \le 7\}$ to satisfy Algorithm 1.1:

1. Choose node c_8 to be equal to any one of $c_1, c_3, c_4, c_5,$ or c_7.
2. Choose the weights $\{\widehat{b}_i, \ i = 1, .., 8\}$, so that
$$\widehat{b}_2 \text{ arbitrary}, \quad \widehat{b}_6 = -\widehat{b}_2, \quad \widehat{b}_8 \neq 0, \text{ arbitrary},$$
$$\sum_{i=1}^{8} \widehat{b}_i c_i^{k-1} = \frac{1}{k}, \quad k = 1, .., 5.$$
3. Now compute $\widehat{B}_j^{[1]} \equiv \sum_{i=j+1}^{8} \widehat{b}_i a_{i,j}$, $j = 1, \ldots, 7$, so that
$$a_{8,6} \text{ is arbitrary}, \ \widehat{B}_6^{[1]} = \widehat{b}_8 a_{8,6} + \widehat{b}_7 a_{7,6}, \ \widehat{B}_2^{[1]} = -\widehat{B}_6^{[1]},$$
$$\sum_{i=1}^{7} \widehat{B}_i^{[1]} c_i^{k-1} = \frac{1}{k(k+1)}, \quad k = 1, .., 4,$$
$$\sum_{i=1}^{7} \widehat{B}_i^{[1]} q_i^{[3]} = 0.$$

4. Finally, compute the coefficients of stage 8 using the substitution formula

$$a_{8,j} = (\widehat{B}_j^{[1]} - \sum_{i=j+1}^{7} \widehat{b}_i a_{i,j})/\widehat{b}_8, \quad j = 1,..,7.$$

Table 5 RK(8-6:5)b: an unreliable 8-stage 6,5 pair of type Hairer [13,22]

0									6
$\frac{1}{6}$	$\frac{1}{6}$								1
$\frac{1}{4}$	$\frac{1}{16}$	$\frac{3}{16}$							3
$\frac{4}{7}$	$\frac{148}{343}$	$-\frac{528}{343}$	$\frac{576}{343}$						3
$\frac{7}{9}$	$-\frac{2849}{17496}$	$\frac{308}{243}$	$-\frac{17024}{19683}$	$\frac{84721}{157464}$					3
$\frac{1}{6}$	$\frac{619}{4200}$	0	$\frac{24}{475}$	$-\frac{147}{2600}$	$\frac{2187}{86450}$				1
1	$\frac{6229}{22120}$	$-\frac{432}{79}$	$\frac{17312}{7505}$	$-\frac{2107}{3160}$	$\frac{39366}{52535}$	$\frac{300}{79}$			3
$\frac{1}{4}$	$-\frac{1}{560}$	$-\frac{293}{144}$	$\frac{16}{95}$	$-\frac{49}{260}$	$\frac{729}{8645}$	$\frac{20}{9}$	0		3
1	$\frac{43}{560}$	$-\frac{1}{3}$	$\frac{2816}{7695}$	$\frac{16807}{84240}$	$\frac{19683}{69160}$	$\frac{1}{3}$	$\frac{79}{1080}$	0	6
1	$\frac{43}{560}$	0	$\frac{4093}{15390}$	$\frac{16807}{84240}$	$\frac{19683}{69160}$	0	$\frac{79}{1080}$	$\frac{1}{10}$	6

In summary, each pair generated by Algorithm 1 is directly determined from the six arbitrary parameters, $\{c_2, c_3, b_2;\ \widehat{b}_2, \widehat{b}_8 \neq 0, a_{8,6}\}$. If $c_2 = 2c_3/3$, one subfamily with $DSO = 3$ is obtained; for this, examples appear in [22], and as Table 5 (for which $c_8 = c_3$).

Another variation of the methods from Algorithm 1.1 occurs by selecting $c_4,\ c_5 = (5 \pm \sqrt{5})/10,\ c_3 = 2c_4/3$. These choices force $a_{4,2} = 0$, and an algorithm analogous to Algorithm 1.2 yields matching methods of order five for any choice of $\widehat{b}_2 \neq b_2$.

For each pair, the coefficients exactly satisfy both sets of order conditions. However, in addition to the 17 conditions up to order 5, the embedded method satisfies all but 4 or 8 of the additional 20 conditions of order six (depending on whether or not $c_8 = c_7$ respectively), and in particular, the quadrature rules are *identical* for both methods. Hence, each pair computed by this pair of algorithms is *unreliable* for adaptive stepsize implementation (see [6], page 209).

4.2 Reliable 6,5 RK pairs

Consider the development of similar algorithms for deriving 7-stage methods of order 6 with the design of those obtained by Khashin in Section 4.1, Example

4.1 [14]. Table 6 below illustrates an 8-stage 6,5 pair with exact coefficients for which stages {2,3,4,5,6} yield DSO=1. Also, stages 1 and 7 have higher stage-order. These pairs are formulated so that the arbitrary parameters may be selected as $\{c_2,\ c_3,\ c_5;\ \widehat{b}_2, a_{8,2}\}$. (Other choices are possible.)

Table 6 RK(8-6,5)c: a reliable 8-stage 6,5 pair of type Khashin [14] 4.1(2)

0									6
$\frac{2}{5}$	$\frac{2}{5}$								1
$\frac{3}{5}$	$\frac{7}{20}$	$\frac{1}{4}$							1
$\frac{1}{7}$	$-\frac{659}{1372}$	$\frac{1431}{1372}$	$-\frac{144}{343}$						1
$\frac{1}{3}$	$\frac{91}{324}$	$\frac{73}{2916}$	$-\frac{1}{162}$	$\frac{49}{1458}$					1
$\frac{17}{23}$	$-\frac{259}{48668}$	$-\frac{10653149}{3358092}$	$\frac{217152}{279841}$	$-\frac{193648}{839523}$	$\frac{943488}{279841}$				1
1	$\frac{1}{6}$	$\frac{4885}{702}$	$-\frac{2855}{1536}$	$\frac{22099}{27648}$	$-\frac{1359}{224}$	$\frac{279841}{279552}$			3
1	$-\frac{5}{4}$	$-\frac{1}{3}$	$-\frac{25293}{4096}$	$-\frac{51401}{122880}$	$\frac{43821}{8960}$	$\frac{1228867}{286720}$	0		1
1	$\frac{1}{12}$	$-\frac{2375}{4212}$	$\frac{2375}{12288}$	$\frac{16807}{663552}$	$\frac{1539}{1792}$	$\frac{6436343}{20127744}$	$\frac{1}{12}$	0	6
1	$\frac{1}{12}$	$-\frac{2375}{16848}$	$-\frac{2375}{98304}$	$\frac{271313}{5308416}$	$\frac{7695}{14336}$	$\frac{67441681}{161021952}$	$\frac{1}{12}$	$-\frac{19}{2304}$	5

Since almost all stage-orders are equal to 1 for these methods, the vector $\mathbf{q^{[2]}}$ has (several) corresponding elements different from zero. For this type of method, the set $\{\mathbf{b}^t, \mathbf{b}^t\mathbf{C}\}$ forms a basis of $\mathcal{L}_2$ that has dimension 2. Since vectors of $\mathcal{R}_4$ lie in $\mathbb{R}^7/\mathbf{e}_1$, the rank theorem implies its dimension is 4. Consider the vectors $\{\mathbf{q}^{[2]}, \mathbf{Cq}^{[2]}, \mathbf{C}^2\mathbf{q}^{[2]}, (\mathbf{q}^{[2]})^2\}$. The first three are linearly independent. It is possible for this set to form a basis of $\mathcal{R}_4$, but for this type of method, the alternative occurs. Indeed, we shall assume that $K_4 = 0$ in (24): it follows for each j with $q_j^{[2]} \neq 0$, that $q_j^{[2]} = K_1 + K_2 c_j + K_3 c_j^2$. Since $c_1 = 0$, $q_1^{[2]} = 0$ identically, and assume (temporarily) that all remaining $q_j^{[2]} \neq 0,\ j = 2, \ldots, 7$. Then, for each $k = 1, 2, 3$, the order conditions require that

$$0 = \sum_{i=1}^{7} b_j c_j^k q_j^{[2]} = \sum_{i=1}^{7} b_j c_j^k (K_1 + K_2 c_j + K_3 c_j^2) = \frac{K_1}{k+1} + \frac{K_2}{k+2} + \frac{K_3}{k+3}. \tag{26}$$

This yields a square non-singular matrix equation in K_j with right side zero. This would imply that $K_1 = K_2 = K_3 = 0$, a contradiction, so that there must be some $j > 1$ with $q_j^{[2]} = 0$. In the methods derived here, we assume $j = 7$ with $c_7 = 1$, and that $q_j^{[2]} \neq 0,\ j = 2, .., 6$ (although other choices may be possible). It also follows that $q_7^{[3]} = 0$ since $\mathbf{q^{[3]}}$ is spanned by $\{\mathbf{q}^{[2]}, \mathbf{Cq}^{[2]}\}$.

Repeating the computation (26) with $q_7^{[2]} = 0$ leads to

$$\frac{K_1}{k+1} + \frac{K_2}{k+2} + \frac{K_3}{k+3} = b_7(K_1 + K_2 + K_3), \quad k = 1, 2, 3, \tag{27}$$

for which the solution is $b_7 = 1/12$, $5K_1 = -K_2 = K_3$. The analogous computation for $k = 0$ yields a similar equation in b_1, which yields the solution, $b_1 = 1/12$. For each method, the value of K_1 depends on c_2: in particular, $q_2^{[2]} = K_1 + K_2 c_2 + K_3 c_2^2$, implies that

$$K_1 = \frac{-c_2^2}{2(5c_2^2 - 5c_2 + 1)}.$$

The corresponding equation for $q_3^{[2]}$ implies that

$$a_{3,2} = \frac{(c_3 - c_2)(c_3 + c_2 - 5c_2c_3)}{2c_2(1 - 5c_2 + 5c_2^2)}.$$

These constraints motivate the algorithms for the next family of pairs.

ALGORITHM 2.1

A 3-parameter family of 7-stage methods of order 6 with DSO=1:

1. For $c_1 = 0,\ c_2,\ c_3,\ c_5$ arbitrary, $c_7 = 1$, choose nodes to lie in [0,1], and so that all (but possibly c_2, c_7) are distinct, and

$$c_4 = \frac{(5c_2c_3 - 1)(5c_2c_3 - c_2 - c_3)}{175c_2^2c_3^2 - 100c_2^2c_3 - 100c_2c_3^2 + 15c_2^2 + 15c_3^2 + 60c_2c_3 - 10c_2 - 10c_3 + 2},$$

   and for $p_4(c) = (c - c_2)(c - c_3)(c - c_4)(c - c_5)$,

$$c_6 = \frac{12\int_0^1 c\, p_4(c)dc - p_4(1)}{12\int_0^1 p_4(c)dc - p_4(1) - p_4(0)}.$$

2. Linear dependence of $A\mathbf{q}^{[2]}$ and $\mathbf{q}^{[3]}$ on $\{\mathbf{q}^{[2]}, \mathbf{C}\mathbf{q}^{[2]}\}$: Choose $a_{2,1} = c_2$. For $a_{3,2}$ obtained above, use stages 2 and 3 to compute constants $F_i,\ G_i,\ i = 1, 2$ by satisfying

$$0 = (F_1 + F_2c_2)q_2^{[2]}$$
$$a_{3,2}q_2^{[2]} = (F_1 + F_2c_3)q_3^{[2]}$$

   and

$$q_2^{[3]} = (G_1 + G_2c_2)q_2^{[2]}$$
$$q_3^{[3]} = (G_1 + G_2c_3)q_3^{[2]}$$

3. Compute $a_{4,2}$ and $a_{4,3}$, using

$$a_{4,2}q_2^{[2]} + a_{4,3}q_3^{[2]} = (F_1 + F_2c_4)q_4^{[2]}$$
$$q_4^{[3]} = (G_1 + G_2c_4)q_4^{[2]}$$

4. Compute constants $K_j,\ j = 1, 2, 3$, so that

$$q_i^{[2]} = K_1 + c_i K_2 + c_i^2 K_3, \quad i = 2, 3, 4.$$

5. Compute values of the homogeneous polynomials $B_i^{[k]}$ as follows:
   (a) $B_1^{[0]} = B_7^{[0]} = 1/12$. Compute $B_i^{[0]},\ i = 2, .., 6$ to satisfy

$$\mathbf{B}^{[0]}\mathbf{C}^{k-1}\mathbf{e} = \frac{1}{k}, \quad k = 1, .., 5.$$

   (The choice of c_6 implies this holds for $k = 6$ as well. Also, since $q_1^{[2]} = q_7^{[2]} = 0$, it follows that

$$\begin{aligned} 0 &= \textstyle\sum_{i=2}^{4} b_i(c_i - c_6)(c_i - c_5)c_i(K_1 + c_i K_2 + c_i^2 K_3) \\ &= \textstyle\sum_{i=1}^{7} b_i(c_i - c_6)(c_i - c_5)c_i q_i^{[2]}, \end{aligned}$$

   and then $\{\mathbf{b}^t\mathbf{C}^k\mathbf{q}^{[2]} = 0,\ k = 1, 2\}$ will imply that $\mathbf{b}^t\mathbf{C}^3\mathbf{q}^{[2]} = 0$.)
   (b) Choose $B_i^{[1]} = B_i^{[0]}(1 - c_i), \quad i = 1, .., 6$.
   (c) Choose $B_i^{[2]},\ i = 1, .., 5$ to satisfy

$$\mathbf{B}^{[2]}\mathbf{C}^{k-1}\mathbf{e} = \frac{(k-1)!}{(k+2)!}, \quad k = 1, .., 4,$$

   and

$$\mathbf{B}^{[2]}(\mathbf{C} - c_5\mathbf{I})\mathbf{q}^{[2]} = 0$$

   .
   (d) Choose $B_i^{[3]},\ i = 1, .., 4$ to satisfy

$$\mathbf{B}^{[3]}\mathbf{C}^{k-1}\mathbf{e} = \frac{(k-1)!}{(k+3)!}, \quad k = 1, .., 3,$$

   and $\mathbf{B}^{[3]}\mathbf{q}^{[2]} = 0$.
6. Observe that $\{b_i = B_i^{[0]},\ i = 1, .., 7\}$, and compute the remaining coefficients $\{a_{i,j},\ i = 5, 6, 7\}$, using the back-substitution formula (15).

This gives a family of methods in which stages 2 to 6 are all of stage order 1, and stage 7 has stage order 3. With each method of this three-parameter family in $\{c_2, c_3, c_5\}$, a two-parameter set of embedded methods of order 5 is obtained by appending one additional stage.

ALGORITHM 2.2

A 5-parameter family of 8-stage RK 6,5 pairs with DSO=1: after choosing the first seven stages $\{b_i, a_{i,j}, c_i,\ 1 \le i \le 7\}$ to satisfy Algorithm 2.1:

1. Choose node $c_8 = 1$.

2. Choose the weights $\{\widehat{b}_i, i=1,..,8\}$, so that

$$\widehat{b}_1 = \widehat{b}_7 = 1/12, \quad \text{with } \widehat{b}_2 \neq b_2, \quad \text{arbitrary},$$
$$\sum_{i=1}^{8} \widehat{b}_i c_i^{k-1} = \frac{1}{k}, \quad k = 1,..,5.$$

3. With $a_{8,2}$ arbitrary, choose $\{a_{8,i},\ i=1,3,..,7\}$, of a new stage 8 to satisfy
   (a)
$$\sum_{j=1}^{7} a_{8,j} = c_8,$$
   (b)
$$\sum_{i=1}^{8} \widehat{b}_i q_i^{[k]} = 0, \quad k = 2,3,4,$$
   (c)
$$\sum_{i>j=1}^{8} \widehat{b}_i a_{i,j} q_j^{[2]} = 0,$$
   (d)
$$\sum_{i>j>k=1}^{8} \widehat{b}_i a_{i,j} a_{j,k} q_k^{[2]} = 0.$$

To illustrate that different approaches to derivation are possible (but not necessary), formulas proposed for solving the order conditions in Algorithm 2 differ slightly from those used in Algorithm 1. Here, we observe that the equations (27) force the same values $\widehat{b}_1 = \widehat{b}_7 = \frac{1}{12}$ as for b_1 and b_7. Some choices of the nodes are excluded ($c_2 = 1/3$ or $c_2 = 1/4$) to ensure that coefficients of a pair can be obtained without encountering an inconsistent system.

Each pair of this family is an improvement over those obtained using Algorithm 1: because every term of order 6 in the series expansion of the error estimate $[y_{n+1} - \widehat{y}_{n+1}]$ has a non-zero coefficient, this error estimate reflects the actual local truncation error of the lower order formula, and so these formulas may be expected to be reliable for implementation with adaptive stepsizes.

5 Reliable 10-stage Runge–Kutta pairs of orders 7 and 6

Parametric families with exact coefficients have been derived for RK 7,6 *pairs* with 10-stages and DSO=3 in [18,19,23], and with 11-stages and DSO=4 in [17]. The two examples of 9-stage *methods* of order 7 in [14] have DSO=2. However, in attempts to derive such methods directly, the tools above have so far only yielded explicit equations for the coefficients that *exactly* satisfy 82 of the 85 order conditions up to order 7. In each method, the choice of $a_{5,4}$ yields a unique value of c_6 giving values of three expressions of order 7:

$$\mathbf{b}^t[\mathbf{q}^{[3]}]^2 \qquad \mathbf{b}^t \cdot \mathbf{q}^{[3]} * \mathbf{A}\mathbf{q}^{[2]} \qquad \mathbf{b}^t[\mathbf{A}\mathbf{q}^{[2]}]^2 \qquad (28)$$

(corresponding to three of the rooted trees each with two articulated branches of height ≥ 2). These three values are continuous in $a_{5,4}$, change signs in an (arbitrarily) small interval $[l_{5,4}, r_{5,4}]$, and because of linear dependence are simultaneously zero at some point of this interval. In practice, exact values of all coefficients are obtained as functions of the arbitrary parameters, and these may be chosen so that values in (28) can be made less than some specified tolerance. In theory, there is a value of node c_6 that may be expressed in terms of the arbitrary parameters that determines that value of $a_{5,4}$ for which (28) are exactly zero, but computations with MAPLE have not (yet) been successful in obtaining an explicit formula for c_6.

ALGORITHM 3.1

A 6-parameter family of 9-stage methods of order 7 with DSO = 2:

1. Choose $\{c_1 = 0,\ c_i,\ i = 2,3,4,5,\ 7,8,$ arbitrary, $c_9 = 1\}$, in [0,1] with $\{c_i,\ i = 1,4,5,6,7,8,9\}$ distinct. (Preserve c_6 as a parameter until the final step of this Algorithm.)
2. As $\langle \mathbf{q}^{[2]} \rangle = \langle [0, -c_2^2/2, 0, \ldots, 0] \rangle$ contains $\{\mathbf{C}^k \mathbf{q}^{[2]}, k = 1, .., (\mathbf{q}^{[2]})^2, (\mathbf{q}^{[2]})^3\}$, we choose $\{\mathbf{q}^{[2]}, \mathbf{q}^{[3]}, \mathbf{q}^{[4]}, \overline{\omega}_4(\mathbf{C})\mathbf{e}, \mathbf{q}^{[5]}, \overline{\omega}_5(\mathbf{C})\mathbf{e}\}$ as a basis for $\mathcal{R}_5$.
3. Choose $a_{2,1} = c_2$, and $a_{3,i}$ to satisfy $\mathbf{q}_3^{[k]} = 0,\ k = 1,2$.
4. Compute F_i so that
$$\mathbf{A}\mathbf{q}^{[2]} = F_1 \mathbf{q}^{[2]} + F_2 \mathbf{q}^{[3]} \tag{29}$$
using stages 2 and 3. Compute $a_{4,i}$ to satisfy (29) and $\{\mathbf{q}_4^{[k]} = 0,\ k = 1,2\}$.
5. *Select* a trial value of $a_{5,4}$. Compute the remaining $a_{5,i}$ to satisfy (29) for stage 5, and $\{\mathbf{q}_5^{[k]} = 0,\ k = 1,2\}$.
6. Compute $H_i,\ J_i$ from stages 2 to 5 so that
$$\mathbf{A}\mathbf{q}^{[3]} = H_1 \mathbf{q}^{[2]} + H_2 \mathbf{q}^{[3]} + H_3 \mathbf{q}^{[4]} + H_4 \overline{\omega}_4(\mathbf{C})\mathbf{e} \tag{30}$$
$$\mathbf{C}\mathbf{q}^{[3]} = J_1 \mathbf{q}^{[2]} + J_2 \mathbf{q}^{[3]} + J_3 \mathbf{q}^{[4]} + J_4 \overline{\omega}_4(\mathbf{C})\mathbf{e} \tag{31}$$
Compute $a_{6,i}$ to satisfy (29)–(31) for stage 6, and $\{\mathbf{q}_6^{[k]} = 0,\ k = 1,2\}$.
7. (a) Choose $B_2^{[0]} = 0$, and compute $\{B_i^{[0]},\ i = 1,3,..,9\}$, to satisfy
$$\mathbf{B}^{[0]}\mathbf{C}^{k-1}\mathbf{e} = \frac{1}{k}, \qquad k = 1,..,7,$$
and
$$\sum_{i=3}^{6} B_i^{[0]}(c_i - 1)(c_i - c_8)(c_i - c_7) q_i^{[3]} = 0.$$
(b) Choose $\ B_i^{[1]} = B_i^{[0]}(1 - c_i), \qquad i = 1,..,8.$
(c) Choose $B_2^{[2]} = 0$, and compute $B_i^{[2]},\ i = 1,3,.,7$ to satisfy
$$\mathbf{B}^{[2]}\mathbf{C}^{k-1}\mathbf{e} = \frac{(k-1)!}{(k+2)!}, \qquad k = 1,..,5,$$

and

$$\sum_{i=3}^{6} B_i^{[2]}(c_i - c_7)q_i^{[3]} = 0.$$

(d) Choose $B_2^{[3]} = 0$, and compute $B_i^{[3]},\ i = 1, 3, .., 6$ to satisfy

$$\mathbf{B}^{[3]}\mathbf{C}^{k-1}\mathbf{e} = \frac{(k-1)!}{(k+3)!}, \qquad k = 1, .., 4,$$

and

$$\sum_{i=3}^{6} B_i^{[3]} q_i^{[3]} = 0.$$

8. Observe that $\{b_i = B_i^{[0]},\ i = 1, .., 9\}$, and compute the remaining coefficients $a_{i,j},\ i = 7, 8, 9$, by back-substitution (15). In this case, c_6 remains a function of the trial value of $a_{5,4}$, and the other coefficients.
9. Finally, solve

$$\sum_{i=3}^{7} b_i(c_i - 1)(c_i - c_8)q_i^{[3]} = 0, \tag{32}$$

for c_6.

The final equation is linear in c_6, and if all arbitrary coefficients are, for example, rational, this algorithm can be executed using exact arithmetic in MAPLE, to get exact coefficients. As already mentioned, a value of $a_{5,4}$ needs to be selected so that the expressions in (28) are small.

ALGORITHM 3.2

A 9-parameter family of 10-stage 7,6 RK pairs with DSO=2: after choosing the first nine stages $\{b_i, a_{i,j}, c_i,\ 1 \le i \le 9\}$ to satisfy Algorithm 3.1:

1. Choose node $c_{10} = 1$.
2. Choose the weights $\{\widehat{b}_i,\ i = 1, .., 10, \}$ so that
   (a)
   $$\widehat{b}_2 = 0, \text{ with } \widehat{b}_3,\ \widehat{b}_{10} \neq 0, \text{arbitrary},$$
   (b)
   $$\sum_{i=1}^{10} \widehat{b}_i c_i^{k-1} = \frac{1}{k}, \quad k = 1, .., 6,$$
   (c)
   $$\sum_{i=1}^{8} \widehat{b}_i (c_i - 1) q_i^{[3]} = 0.$$
3. With $a_{10,8}$ arbitrary, choose $a_{10,i},\ i = 1, 3, .., 9$, of a new stage 10 to satisfy
   (a)
   $$\sum_{j=1}^{9} a_{10,j} = c_{10},$$
   (b)
   $$\sum_{i=2}^{10} \widehat{b}_i q_i^{[k]} = 0, \quad k = 2, .., 5,$$

(c)

$$\sum_{i>j=2}^{10} \widehat{b}_i a_{i,j} q_j^{[2]} = 0,$$

(d)

$$\sum_{i>j=2}^{10} \widehat{b}_i c_i^k q_i^{[3]} = 0, \quad k = 1, 2.$$

Selecting the arbitrary parameters from either Example 2. or 3. from Section 4.2 of [14] yields the coefficients for both methods displayed.[5] Coefficients for each *method* are functions of the 6 arbitrary nodes, $\{c_2, c_3, c_4, c_5, c_7, c_8\}$. (For each of these methods, there is a 3-parameter family of embedded methods depending on values of $\{\widehat{b}_3, \widehat{b}_{10}, a_{10,8}\}$.)

Choosing nodes $\mathbf{c} = [0, 1/30, 1/18, 1/8, 3/10, c_6, 7/10, 4/5, 1, 1]$, and $a_{5,4} = 1526429125535309/2000000000000000$ gives

$$c_6 = \frac{10408718373744539857431009846 07238}{31463500513723651766453260903262 85},$$

and the coefficients of the pair exactly satisfy all but three order conditions to order 7: only each term of (28) is approximately zero, and for this method, $||T_7||_2 \approx 1.11(10)^{-21}$ and error norm $||T_8||_2 \approx 6.42(10)^{-5}$. Moreover, each matched method from Algorithm 3.2 exactly satisfies all order conditions up to order 6. On coding Algorithm 3, a pair with these coefficients may be obtained. What is remarkable is that c_6 is determined *linearly* from (32) in the arbitrary parameters: unfortunately an explicit algebraic expression for c_6 (currently) remains unknown.

6 Conclusions

In a search for better algorithms for the efficient approximation of solutions to initial value problems, analysis of the structure and derivation of new Runge–Kutta methods can be helpful. Here, we have extended some new methods recently derived in [14] and as well, the structure used for their derivation. In particular, this extension allows the construction of embedded matched methods of order $p - 1$ with one additional stage.

It is expected that higher order Runge–Kutta pairs of similar structure can be represented using this approach, and that the tools developed for solving the order conditions can be applied to the derivation of other types of methods, and may lead to more effective algorithms. It might be hoped that the techniques proposed here will stimulate continuing interest in the quest for better algorithms for treating initial value ordinary differential equations.

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[5] Missing coefficients of Example 2 in [14] are $a_{8,2} \approx 0.813220953152450409411$ and $b_9 \approx 0.0645729382008434924977$.

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