A CLASSIFICATION SCHEME FOR STUDYING EXPLICIT RUNGE-KUTTA PAIRS

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Abstract

Pairs of explicit Runge-Kutta methods of different orders of accuracy form efficient algorithms for treating non-stiff ordinary differential equations. While parametric families of different types and orders are known, the characterization of pairs of orders $p-1$ and $p,\ p \geq 6$, remains incomplete, and the search for better pairs continues.

A scheme to distinguish between pairs of different types has been developed after studying a variety of known methods and pairs. The resulting classification scheme includes almost all known pairs in a natural way, and provides designs which lead to new pairs of several types. To derive a new family of pairs, a promising design is selected from the classification, and the corresponding order equations are solved by adapting or generalizing simplifying conditions that previously facilitated the construction of pairs of a more restricted design. In addition to motivating and describing the classification scheme, examples of some new pairs are given.

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1. **Introduction**

The problem of interest is a vector initial value problem

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

which has a unique solution if f: $\mathbf{R} \times \mathbf{R^N} \to \mathbf{R}$ is Lipschitz continuous in y: $\mathbf{R^N} \to \mathbf{R^N}$. For many acceptable functions f, even if f is a function of t alone, it might not be possible to represent the solution exactly in terms of elementary functions. Often the solution of the restricted problem

$$(1') \qquad y' = f(t), \qquad y_0 = y(t_0).$$

(equivalently, a definite integral) may be approximated recursively at a sequence of points $t_0, t_1, ...$ by a *quadrature rule* of the form

$$(2) \qquad y(t_n+h) = y(t_n) + \int_0^h f(t_n+st)ds \approx y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(t_n+c_ih), \quad n = 0,1,....$$

Usually, the nodes $\{c_i, i = 1,..,s\}$ and the weights $\{b_i, i = 1,..,s\}$ are selected so that (2) is exact whenever y is a polynomial of some specified degree p. Equivalently, the nodes and weights are selected to satisfy the *quadrature conditions*

$$(3) \qquad Q_\tau \equiv \sum_{i=1}^{s} b_i c_i^{\tau-1} - \frac{1}{\tau} = 0, \qquad \tau = 1,..,p.$$

For certain choices of the nodes, these can be satisfied for p as large as $2s-1$, and otherwise for any s nodes of which p are distinct, (3) can be satisfied for any $s \geq p$. If $p = s$, then (3) uniquely determine the weights; otherwise, $s-p$ weights may be chosen arbitrarily. This perspective helps to motivate a strategy for deriving explicit Runge-Kutta methods.

For the more general problem (1), an explicit Runge-Kutta method propagates an approximation y_{n+1} to $y(x_n+h)$ from step-to-step by

$$(4) \qquad y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f_{ni} \quad n = 0,1,....$$

where approximations to corresponding derivative values are given by

$$(4') \qquad f_{ni} = f(t_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} f_{nj}), \qquad i = 1, .., s.$$

The error may be estimated as the difference between y_{n+1} and

$$(5) \qquad \hat{y}_{n+1} = y_n + h \sum_{i=1}^{s} \hat{b}_i f_{ni} \ .$$

For a single method defined by (4) and (4′), the coefficients are selected primarily to maximize its order of accuracy p; if an error estimator is used, the coefficients and the additional weights are further constrained so that (5) has order of accuracy $p-1$. In either case, some parameters can be selected arbitrarily, and hence a *family* of methods or pairs of methods may be found to satisfy the order conditions. In implementing a pair of formulas, either may be used to advance the approximation from step to step. The design of some pairs depends on which choice is to be made, and this is indicated later. For others, the structure of the method is independent which approximation is propagated, and accordingly no attempt has been made to assign or recommend such a choice.

Since Kutta [17] characterized a *family* of fifth order methods in 1901, different types of methods of moderate and high orders have been proposed in the literature. More recently, families of *pairs* of methods requiring a minimum (or near minimum) number of derivative evaluations have been derived by Fehlberg [14], Butcher [4], Verner [32], and Prince and Dormand [23]. Yet, the characterization even for pairs of methods of order $p = 6$ requiring eight stages remains incomplete. Some efforts have been made to improve this situation. Verner [34] determined explicit formulas which directly relate three known families of methods. In other recent work, Sharp [29] develops new pairs of low orders.

This article describes a tool that has been fruitful in the derivation of other new pairs (and as well the construction of interpolants [37,30]) of Runge-Kutta methods. First, approaches that have contributed to the solution of the order equations are contrasted by reviewing various methods and pairs of methods. Observed similarities and differences allow for pairs of methods to be separated into different *classes*. While this classification scheme does not naturally include all types of pairs examined, it has improved our understanding of the basic design in many known pairs, and as a result, led to the construction of some new types of pairs. Other new pairs are currently under development. The immediate benefit of this approach is a more complete characterization of Runge-Kutta pairs. It is also possible that this approach will be more broadly applicable, for example, for constructing explicit general linear methods, and therefore will be of wider general interest.

In the next section, the quadrature equations (3) provide a useful perspective for analyzing various elements of the structure of Runge-Kutta methods. By separating different types of order equations, strategies for deriving new methods are proposed. Section 3 emphasizes differences in the underlying structures of some single methods. Section 4 contrasts the structures of some known error-estimating pairs of methods. The classification scheme and its aspects are described in Section 5. Finally, examples of some new types of methods are given in illustration.

2. **Quadratures and Sub-quadratures**

It is convenient to interpret the Runge-Kutta formula (4) as an extension to (2) in which $y(t_n + c_i h), i = 1, .., s$, is estimated recursively by an internal sub-quadrature rule:

$$y_{ni} = y_n + h \sum_{j=1}^{i-1} a_{ij} f(t_n + c_j h, y_{nj}), \qquad i = 1, .., s, \tag{6}$$

for $c_1 = 0$ and $y_{n1} = y_n$. Accordingly, the *linking coefficients* $\{a_{ij} = 0,\ 1 \leq j < i \leq s\}$ may be determined using certain *sub-quadrature* expressions

$$q_i^\tau \equiv \sum_{j=1}^{i-1} a_{ij} c_j^{\tau-1} - \frac{c_i^\tau}{\tau}, \qquad i = 1, .., s, \qquad \tau = 1, .., p-1. \tag{7}$$

In particular, most methods are constructed so that these coefficients satisfy the sub-quadrature conditions

$$q_i^\tau = 0, \qquad i = 1, .., s, \qquad \tau = 1, .., p_i, \tag{7'}$$

for a certain integer vector of *stage-orders*, $SOV = (p_1, p_2, .., p_s)$. In this article, we require more: stage i will have stage-order p_i if the linking coefficients satisfy both (7′) and the *stage suppressing* conditions

$$a_{ij} = 0, \qquad p_i > p_j + 1. \tag{7''}$$

Further, it is convenient to append the *quadrature* orders p and $p-1$ of the approximating stages (4) and (5) to these SOVs usually following a colon to give an augmented stage-order vector (ASOV). For methods in which an approximating stage is "reused", its quadrature order will be included in the basic SOV. For example, a method with ASOV=(5,1,2,2,2,2:5,4) (equivalently (5,1,2,2,2,2:4,5)) requires six stages to give two independent approximations of orders 4 and 5, whereas one with ASOV=(5,1,2,2,2,2,5:4) requires the first six stages to give an approximation of order 5, and all seven of these stages to give the additional approximation of order 4. Often, but not necessarily, these quadrature orders will be the orders of the approximating stages.

Also, it is usually convenient to display the nodes, weights and linking coefficients of an explicit Runge-Kutta method in the format of a Butcher tableau.

Tableau 1: A Butcher Tableau

c_1							
c_2	a_{21}						
c_3	a_{31}	a_{32}					
.	.	.	.				
.	.	.	.	.			
c_s	a_{s1}	a_{s2}	.	.		$a_{s,s-1}$	
$\mathbf{b}^p$	b_1	b_2	.	.		.	b_s

For an error-estimating pair, the weights of (5) will be appended to this table. To obtain a method of order p, the coefficients must be chosen to satisfy the algebraic order conditions, and these may be most conveniently enumerated using a one-to-one mapping onto the set of rooted trees developed by Butcher[1]. For $p \geq 5$, s internal stages with $s > p$ are needed [3], and the order equations can be separated into four different groups. Using (3) and (7), the groups for $p = 5$ illustrate this separation.

5 Quadrature equations:

$$\sum_{i=1}^{s} b_i c_i^{\tau-1} - \frac{1}{\tau} = 0, \qquad \tau = 1, .., 5, \tag{3}$$

6 Basic sub-quadrature equations

$$\sum_{i=1}^{s} b_i \{ \sum_{j=1}^{i-1} a_{ij} c_j^{\tau-1} - \frac{c_i^{\tau}}{\tau} \} = 0, \qquad \tau = 2, 3, 4, \tag{8'}$$

$$(8'') \qquad \sum_{i=1}^{s} b_i \sum_{j=1}^{i-1} a_{ij} \{ \sum_{k=1}^{j-1} a_{jk} c_k^{\tau-1} - \frac{c_j^\tau}{\tau} \} = 0, \qquad \tau = 2, 3,$$

$$(8''') \qquad \sum_{i=1}^{s} b_i \sum_{j=1}^{i-1} a_{ij} \sum_{k=1}^{j-1} a_{jk} \{ \sum_{l=1}^{k-1} a_{kl} c_l - \frac{c_k^2}{2} \} = 0,$$

5 Extended sub-quadrature equations

$$(9') \qquad \sum_{i=1}^{s} b_i c_i^\sigma \{ \sum_{j=1}^{i-1} a_{ij} c_j^{\tau-1} - \frac{c_i^\tau}{\tau} \} = 0, \qquad \sigma \geq 1, \qquad \tau \geq 2, \qquad \sigma + \tau \leq 4,$$

$$(9'') \qquad \sum_{i=1}^{s} b_i c_i^\nu \sum_{j=1}^{i-1} a_{ij} c_j^\tau \{ \sum_{k=1}^{j-1} a_{jk} c_k - \frac{c_j^2}{2} \} = 0, \qquad \nu + \tau = 1,$$

1 Nonlinear sub-quadrature equation

$$(10) \qquad \sum_{i=1}^{s} b_i \{ \sum_{j=1}^{i-1} a_{ij} c_j - \frac{c_i^2}{2} \}^2 = 0.$$

In this formulation, sub-quadratures are explicit in all but the quadrature conditions (3). This indicates why a choice of coefficients which makes low-order sub-quadrature expressions equal to zero can help to minimize the number of stages required.

While Butcher's elegant characterization of the order conditions has been known for some time, their solution for $p \geq 6$ is still incomplete. Nevertheless, most known methods can be derived by solving each group of equations separately, although not independently. In an analogous way that p weights may be chosen to satisfy the quadrature conditions (3), certain homogeneous polynomials of low degree in the linking coefficients may be selected to satisfy the basic sub-quadrature conditions (8). Low order sub-quadrature expressions and the remaining homogeneous polynomials in the linking coefficients are chosen equal to zero, and some constraints are placed on the nodes in order to satisfy the remaining equations. Some detail in solving (8) appears in §3, and [35,39] use this approach to derive some pairs of design order $p \geq 6$.

3. The Structure of Some Single Methods

Here, we shall consider the design of methods of several orders for which a minimum or near minimum number of stages is required. For many methods, particularly those of orders $p \geq 5$, the stage-order vector is a determining factor in the number of stages required. Hence, in representing each method as a Butcher tableau an appended column specifies the augmented stage-order vector.

For example, Euler's method [12] is represented by

Tableau 2: The Euler method

0		|	1
$\mathbf{b}^1$	1	|	1

In 1895, Runge [24] developed a pair of methods, each of order 2, which he suggested could be used to approximate the solution and estimate the error, respectively.

Tableau 3: A pair of methods designed by Runge

0			|	2
$\frac{1}{2}$	$\frac{1}{2}$		|	1
$\mathbf{b}^2$	0	1	|	2

0				|	2
1	1			|	1
1	0	1		|	1
$\mathbf{b}^2$	$\frac{1}{2}$	0	$\frac{1}{2}$	|	2

By 1905, he had extended this treatment [25] to consider *the* widely-publicized method of order 4:

Tableau 4: The Runge-Kutta method

0					|	4
$\frac{1}{2}$	$\frac{1}{2}$				|	1
$\frac{1}{2}$	0	$\frac{1}{2}$			|	1
1	0	0	1		|	1
$\mathbf{b}^4$	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$	|	4

In the interim, Kutta [17] showed that coefficients of methods up to order 5 could be represented parametrically, and had constructed a family of six-stage methods of this order. He selected two particular methods of this family for display.

Tableau 5: Two order 5 methods designed by Kutta

0							5
$\frac{1}{5}$	$\frac{1}{5}$						1
$\frac{2}{5}$	0	$\frac{2}{5}$					2
1	$\frac{9}{4}$	-5	$\frac{15}{4}$				2
$\frac{3}{5}$	$-\frac{63}{100}$	$\frac{9}{5}$	$-\frac{13}{20}$	$\frac{2}{25}$			2
$\frac{4}{5}$	$-\frac{18}{75}$	$\frac{4}{5}$	$\frac{2}{15}$	$\frac{8}{75}$	0		2
$\mathbf{b}^5$	$\frac{17}{144}$	0	$\frac{100}{144}$	$\frac{2}{144}$	$-\frac{50}{144}$	$\frac{75}{144}$	5

0							5
$\frac{1}{3}$	$\frac{1}{3}$						1
$\frac{2}{5}$	$\frac{4}{25}$	$\frac{6}{25}$					2
1	$\frac{1}{4}$	-3	$\frac{15}{4}$				2
$\frac{2}{3}$	$\frac{2}{27}$	$\frac{10}{9}$	$-\frac{50}{81}$	$\frac{8}{81}$			2
$\frac{4}{5}$	$\frac{2}{25}$	$\frac{12}{25}$	$\frac{2}{15}$	$\frac{8}{75}$	0		2
$\mathbf{b}^5$	$\frac{23}{192}$	0	$\frac{125}{192}$	0	$-\frac{27}{64}$	$\frac{125}{192}$	5

The presence of errors in both tables of [17] indicates that even for $p = 5$, solution of the order equations is not a trivial exercise. This family of methods have two features common to high-order explicit methods: both $b_2 = 0$, and $s > p$ for orders $p > 4$. In contrast, another feature common to the Kutta methods, namely $a_{65} = 0$, does not occur in more recent methods. While additional imbedded approximations of order 4 can be constructed for each member of this family, the error estimator that would be obtained is somewhat unreliable. Nevertheless, the generality of Kutta's formulation was a substantial contribution particularly as it appeared so early in the development of these methods.

It wasn't until the $1950's$ that Konen and Luther [16,18,19] completed the classification of methods of order 5 with $b_2 = 0$. Even so, more methods of order 5 for which $b_2 \neq 0$ were subsequently constructed by Cassity [6]. Other methods with $b_2 \neq 0$ rely on selecting some nodes to be equal. Indeed, it appears likely that Cassity's methods may be the only minimal stage methods with $b_2 \neq 0$ for which the nodes are all distinct. Observe that since $q_2^2 \neq 0$, equation (10) implies that at least one of the weights must be negative. Further, since there are six non-zero weights, one weight may be chosen independently of the quadrature conditions (3).

Tableau 6: A Cassity method of order 5 with $b_2 \neq 0$

0							5
$\frac{1}{7}$	$\frac{1}{7}$						1
$\frac{5}{14}$	$-\frac{367}{4088}$	$\frac{261}{584}$					1
$\frac{9}{14}$	$\frac{41991}{2044}$	$-\frac{2493}{73}$	$\frac{57}{4}$				1
$\frac{6}{7}$	$-\frac{108413}{196224}$	$\frac{58865}{65408}$	$\frac{5}{16}$	$\frac{265}{1344}$			1
1	$-\frac{204419}{58984}$	$\frac{143829}{58984}$	$\frac{171}{202}$	$\frac{2205}{404}$	$-\frac{432}{101}$		1
$\mathbf{b}^5$	$\frac{1}{9}$	$\frac{7}{2700}$	$\frac{413}{810}$	$\frac{7}{450}$	$\frac{28}{75}$	$-\frac{101}{8100}$	5

Another observation is basic to the structure of most methods displayed. For such a method, all stages with non-zero weights (except the first), have the *same* stage-order. Since these stages are foremost in the propagation of a solution, we shall designate their order as the *dominant stage-order* (DSO) of a method. For example, DSO=2 for the Kutta methods, and DSO=1 for the Cassity methods. For many, but not all, minimum stage methods of orders $p \geq 5$, the DSO is either $p-3$ or $p-4$.

Further, many methods may be constructed using homogeneous polynomials of the coefficients defined by $B_{1i} = b_i, i = 1, .., s$, and

(11) $$B_{rj} = \sum_{i=j+1}^{s+2-r} B_{r-1,i} a_{ij}, \qquad j = 1, .., s+1-r, \qquad r = 2, .., \rho,$$

for some $\rho \leq p$. Consider, for example, the Kutta methods with DSO=2. Only $q_2^2 \neq 0$.

Hence, equations (3) and (8) including q_i^2 imply that

$$\sum_{i=2}^{s+1-r} B_{r,i} q_i^2 = 0, \qquad r = 1,..,3, \tag{12}$$

or equivalently $b_{12} = B_{22} = B_{32} = 0$. Further, just as equations (3) uniquely determine the weights, the basic sub-quadrature equations (8) uniquely determine the *remaining* homogeneous polynomials for this method. For example, with $s = 6, p = 5$, $\{B_{31}, B_{33}, B_{34}\}$ are uniquely determined to satisfy ($8''$) rewritten in the form

$$\sum_{i=1}^{4} B_{3i} c_i^{\tau-1} = \frac{1}{\tau(\tau+1)(\tau+2)}, \qquad \tau = 1, 2, 3. \tag{13}$$

These choices also satisfy some of the conditions in (9) and (10); others are satisfied by suitable constraints on the nodes. After choosing coefficients $\{a_{ij}, i = 1,..,s+1-\rho\}$ to satisfy ($7'$) and ($7''$) for an appropriate augmented stage-order vector, homogeneous polynomials chosen to satisfy analogs of (12) and (13) may be used recursively with (11) to determine the remaining coefficients. In methods and pairs yet to be examined, it will often be observed that $p = DSO + \rho$ where ρ is the highest degree of homogeneous polynomials computed by equations analogous to (13).

Tableau 7: A Butcher seven-stage method of order 6

0								6
$\frac{5\mp\sqrt{5}}{10}$	$\frac{5\mp\sqrt{5}}{10}$							1
$\frac{5\pm\sqrt{5}}{10}$	$\frac{\mp\sqrt{5}}{10}$	$\frac{5\pm2\sqrt{5}}{10}$						2
$\frac{5\mp\sqrt{5}}{10}$	$\frac{-15\pm7\sqrt{5}}{20}$	$\frac{-1\pm\sqrt{5}}{4}$	$\frac{15\mp7\sqrt{5}}{10}$					2
$\frac{5\pm\sqrt{5}}{10}$	$\frac{5\mp\sqrt{5}}{60}$	0	$\frac{1}{6}$	$\frac{15\pm7\sqrt{5}}{60}$				3
$\frac{5\mp\sqrt{5}}{10}$	$\frac{5\pm\sqrt{5}}{60}$	0	$\frac{9\mp5\sqrt{5}}{12}$	$\frac{1}{6}$	$\frac{-5\pm3\sqrt{5}}{10}$			3
1	$\frac{1}{6}$	0	$\frac{-55\pm25\sqrt{5}}{12}$	$\frac{-25\mp7\sqrt{5}}{12}$	$5\mp2\sqrt{5}$	$\frac{5\pm\sqrt{5}}{2}$		3
$\mathbf{b}^6$	$\frac{1}{12}$	0	0	0	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{12}$	6

While several eight-stage methods of order 6 are known, Butcher [2] was the first to construct such a method requiring only seven stages. His strategy exploits certain *simplifying* assumptions which reduce the total number of algebraic equations to be solved. This approach in tandem with his scheme for enumeration of the order conditions prevail in most strategies for solving the order conditions. He observes that the particular method "is interesting in that it is an explicit counterpart of a certain four-stage implicit process ... the possibility is naturally suggested that counterparts exist for higher order implicit processes as well." For this method, we observe that the DSO=3. Also seven-stage methods with the DSO=2 exist, and an example is included later.

Butcher's challenge was taken up by Cooper, and Curtis independently, each of whom constructed eleven-stage methods of order 8 based on the five-node Lobatto quadrature rule. Cooper and Verner [7] establish the existence of a discrete set of methods of arbitrary order $p \geq 8$ requiring $(p^2 - 7p + 14)/2$ stages. Curtis [8] characterized a four-parameter family of eleven-stage methods of order 8, and subsequently [9] found eighteen-stage methods of order 10. Verner [31] later showed that methods of the Curtis type existed with $p \geq 12$ requiring $(p^2 - 12p + 58)/2$ stages.

Tableau 8: Template for Cooper-Verner eleven-stage methods of order 8

$\ell_0 = 0$											8
$\ell_2 = .5$	X										1
ℓ_2	X	X									2
ℓ_1	X	X	X								2
ℓ_1	X	0	X	X							3
ℓ_2	X	0	X	X	X						3
ℓ_3	X	0	X	X	X	X					3
ℓ_3	X	0	0	0	X	X	X				4
ℓ_2	X	0	0	0	X	X	X	X			4
ℓ_1	X	0	0	0	X	X	X	X	X		4
$\ell_4 = 1$	X	0	0	0	X	X	X	X	X	X	4
$\mathbf{b}^8$	ω_0	0	0	0	0	0	0	ω_3	ω_2	ω_1 ω_4	8

The stage-order vectors and the patterns of zero coefficients and weights for the two methods of order 8 are of interest. For each, $DSO = 4$. Nodes and weights of a Lobatto rule are denoted by $\{\ell_i, i = 0, .., 4\}$ and $\{\omega_i, i = 0, .., 4\}$, and non-zero coefficients by X. In the Curtis methods, some nodes (A for arbitrary, X for non-zero) need not be Lobatto nodes. The patterns are sufficiently different to distinguish the methods as members of two non-intersecting families. Yet, for both methods, weights corresponding to sub-dominant stages are all equal to zero. This property is not necessary even in methods of higher orders.

Tableau 9: Template for Curtis eleven-stage methods of order 8

$\ell_0 = 0$												8
A	X											1
X	X	X										2
X	X	0	X									3
A	X	0	X	X								3
ℓ_3	X	0	0	X	X							4
ℓ_1	X	0	0	X	X	X						4
ℓ_2	X	0	0	X	X	X	X					4
ℓ_3	X	0	0	X	X	X	X	X				4
ℓ_1	X	0	0	X	X	X	X	X	X			4
$\ell_4 = 1$	X	0	0	X	X	X	X	X	X	X		4
$\mathbf{b}^8$	ω_0	0	0	0	0	ω_3	ω_1	ω_2	ω_3	ω_1	ω_4	8

Indeed, the theme of reducing the number of stages to achieve a particular order has another facet. Hairer[15] derived seventeen-stage methods of order 10. His construction relied on counterbalancing a non-zero value of b_2 by choosing $c_2 = c_{16}$ and $b_2 + b_{16} = 0$. Analogous conditions were required of stages 3, 6 and 7. The nodes and weights focus on those of a six-node Lobatto quadrature rule, with other nodes being determined by supplementary orthogonality conditions. Six arbitrary parameters are subscripted by A, and one more is utilized to satisfy a particular constraint of order 11. Non-zero coefficients are denoted by X and Y with the latter identifying coefficients which lead to special cancellations. These and other coefficients equal to zero in Tableau 10 indicate much of the structure of this seven-parameter family of methods. A significant feature in this family is the fact that the stage-order vector initially increases to p-5, and then *decreases* to 1. This is in distinct contrast to each previous type in which the SOV is increasing. In the next section, a related method of order 6 is displayed.

Tableau 10: Template for Hairer seventeen-stage methods of order 10

$\ell_0 = 0$																		10
P_A	X																	1
Q	X	Y																2
X	X	0	X															3
X	X	0	X	X														3
R_A	X	0	0	Y	Y													4
S	X	0	0	Y	Y	X												4
X	X	0	0	0	X	X	X											4
ℓ_2	X	0	0	0	0	X	X	X										5
ℓ_4	X	0	0	0	0	X	X	X	X									5
ℓ_3	X	0	0	0	0	X	X	X	X	X								5
ℓ_1	X	0	0	0	0	X	X	X	X	X	X							5
R	X	0	0	Y	Y	X	X	X	X	X	X	X						4
S	X	0	0	Y	Y	X	X	X	X	X	X	X	X					4
Q	X	Y	0	0	0	Y	Y	0	0	0	0	0	Y	Y				2
P	X	0	Y	0	0	0	0	0	0	0	0	0	0	0	Y			1
$\ell_5 = 1$	X	Y	Y	0	0	X	X	X	X	X	X	X	X	X	Y	Y		5
$\mathbf{b}^{10}$	ω_0	$-p$	$-q$	0	0	$-r$	$-s$	0	ω_2	ω_4	ω_3	ω_1	r_A	s_A	q_A	p_A	ω_5	10

4. The Development of Runge-Kutta Pairs

While strategies for deriving methods of moderate and high order evolved, the need for simultaneous error estimates gained prominence. For Runge-Kutta methods, pairs of approximations of different (usually adjacent) orders of accuracy provide the most efficient algorithms. Early attempts to derive such pairs were unduly influenced by the difficulty in satisfying the necessary order constraints (essentially duplicated for the two methods). Five-stage methods of design order 4 obtained by Merson [20] and Scraton [28] were of order four only for certain problems. Fehlberg [13], Sarafyan [27] England [11] were early developers of some six-stage pairs of orders 4 and 5. However, the major impetus to this area of development was Fehlberg's derivation [14] of pairs of orders $p-1$ and p for $p = 6, 7, 8, 9$. By choosing two nodes $c_1 = c_{s-1} = 0$ for a method of order p, and appending one additional stage at $c_{s+1} = 1$, he derived a 'matched' method of order $p-1$. Pairs in which both approximations use only the initial s stages are denoted by (s, p-1:p), and a pair selected by Fehlberg follows.

Tableau 11: A Fehlberg (8, 5:6) pair

0									6
$\frac{1}{6}$	$\frac{1}{6}$								1
$\frac{4}{15}$	$\frac{4}{75}$	$\frac{16}{75}$							2
$\frac{2}{3}$	$\frac{5}{6}$	$-\frac{8}{3}$	$\frac{5}{2}$						2
$\frac{4}{5}$	$-\frac{8}{5}$	$\frac{144}{25}$	-4	$\frac{16}{25}$					2
0	$-\frac{11}{640}$	0	$\frac{11}{256}$	$-\frac{11}{160}$	$\frac{11}{256}$				3
1	$\frac{93}{640}$	$-\frac{18}{5}$	$\frac{803}{256}$	$-\frac{11}{160}$	$\frac{99}{256}$	1			2
1	$\frac{361}{320}$	$-\frac{18}{5}$	$\frac{407}{128}$	$-\frac{11}{80}$	$\frac{55}{128}$	0	0		2
$\mathbf{b}^6$	$\frac{7}{1408}$	0	$\frac{1125}{2816}$	$\frac{9}{32}$	$\frac{125}{768}$	$\frac{5}{66}$	$\frac{5}{66}$	0	6
$\mathbf{b}^5$	$\frac{31}{384}$	0	$\frac{1125}{2816}$	$\frac{9}{32}$	$\frac{125}{768}$	0	0	$\frac{5}{66}$	6

While this derivation was a substantial advance, each method constructed was deficient in treating the quadrature problem ($1'$) (and any problem containing a quadrature component) – the error estimate is zero while the error may be nonzero. In response to a need for error-estimating pairs without this deficiency, two types of formulas of a different design were derived.

Tableau 12: A Butcher (9*, 5(6)) pair

0						6
$\frac{2}{27}$	$\frac{2}{27}$			$r = \sqrt{2769}$		1
$\frac{1}{9}$	$\frac{1}{36}$	$\frac{1}{12}$				3
$\frac{1}{6}$	$\frac{1}{24}$	0	$\frac{1}{8}$			3
$\frac{1}{3}$	$\frac{1}{6}$	0	$-\frac{1}{2}$	$\frac{2}{3}$		3
$\frac{1}{2}$	$\frac{15}{8}$	0	$-\frac{63}{8}$	7	$-\frac{1}{2}$	3
$\frac{2}{3}$	$\frac{2269-49r}{1164}$	0	$\frac{-6545+141r}{776}$	$\frac{4491-91r}{582}$	$\frac{-2175+35r}{2328}$	
		$\frac{215+r}{582}$				3
$\frac{5}{6}$	$\frac{446107-7484r}{1164}$	0	$\frac{-131141+2256r}{776}$	$\frac{213494-3818r}{18165}$	$\frac{-12381+617r}{18165}$	
		$\frac{-6436-138r}{18165}$	$\frac{16173+89r}{36330}$			3
$\mathbf{b}^5$	$\frac{73-11r}{1020}$	0	0	$\frac{-3054+55r}{1020}$	$\frac{3258-55r}{510}$	
		$\frac{-2952+55r}{510}$	$\frac{2901-55r}{1020}$	$\frac{-162+11r}{1020}$		5
$\mathbf{b}^6$	$\frac{78-r}{390}$	0	0	$\frac{-169+4r}{260}$	$\frac{299-5r}{130}$	
		$\frac{-1053+20r}{390}$	$\frac{299-5r}{260}$	$\frac{-1692+4r}{260}$	$\frac{78-r}{390}$	6

In pairs designed by Butcher [4], the approximation of lower order is computed first. Then the original stages and the derivative evaluation of the first approximation are used to compute the approximation of higher order. For example, for the pair of orders 5 and 6 in Tableau 12, nine stages are needed. The ninth stage may be reused in the first stage of the next step *if the fifth order approximation is propagated.* This design is denoted here and later by placing the order of the approximation requiring the extra stage in parentheses, and placing an asterisk on the total number of stages.

In contrast, the methods of the type displayed in Tableau 13 need only eight stages for approximations of both orders 5 an 6. Because the latter formula required fewer stages, it appeared to be more efficient at least superficially, and methods of this type have been adopted as the basis for some general purpose software. However, recent testing [36] as well as the improvement in selection of particular pairs [23,29] indicates that a more careful selection process is warranted.

Tableau 13: A Verner (8, 5:6) pair

0									6
$\frac{1}{6}$	$\frac{1}{6}$								1
$\frac{4}{15}$	$\frac{4}{75}$	$\frac{16}{75}$							2
$\frac{2}{3}$	$\frac{5}{6}$	$-\frac{8}{3}$	$\frac{5}{2}$						2
$\frac{5}{6}$	$-\frac{165}{64}$	$\frac{55}{6}$	$-\frac{425}{64}$	$\frac{85}{96}$					2
$\frac{1}{15}$	$-\frac{8263}{15000}$	$\frac{124}{75}$	$-\frac{643}{680}$	$-\frac{81}{250}$	$\frac{2484}{10625}$				2
1	$\frac{3501}{1720}$	$-\frac{300}{43}$	$\frac{297275}{52632}$	$-\frac{319}{2322}$	$\frac{24068}{84065}$	$\frac{3850}{26703}$			2
1	$\frac{12}{5}$	-8	$\frac{4015}{612}$	$-\frac{11}{36}$	$\frac{88}{255}$	0	0		2
$\mathbf{b}^6$	$\frac{3}{40}$	0	$\frac{875}{2244}$	$\frac{23}{72}$	$\frac{264}{1955}$	$\frac{125}{11592}$	$\frac{43}{616}$	0	6
$\mathbf{b}^5$	$\frac{13}{160}$	0	$\frac{2375}{5984}$	$\frac{5}{16}$	$\frac{12}{85}$	0	0	$\frac{3}{44}$	5

Tableau 14: A Hairer (8, 5:6) pair

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
1	$\frac{857}{4424}$	$-\frac{132}{79}$	$\frac{102816}{40527}$	$-\frac{7595}{8216}$	$\frac{118098}{136591}$	0	0		3
$\mathbf{b}^6$	$\frac{43}{560}$	$-\frac{1}{3}$	$\frac{2816}{7695}$	$\frac{16807}{84240}$	$\frac{19683}{69160}$	$\frac{1}{3}$	$\frac{79}{1080}$	0	6
$\mathbf{b}^5$	$\frac{43}{560}$	0	$\frac{2816}{7695}$	$\frac{16807}{84240}$	$\frac{19683}{69160}$	0	0	$\frac{79}{1080}$	6

Other eight-stage pairs of orders 5 and 6 exist. A special type [33] based on the design proposed by Hairer [15] is displayed in Tableau 14. For this pair, a suitable choice for the DSO is not obvious. There are two stages of stage-order 1 with non-zero weights. Because these weights sum to zero, this could be accommodated by relaxing the definition of stage-order. On the other hand, the remaining stages satisfy (7′), but not (7′′) for $p_i = 3$. In other methods of this design, the choice $c_2 \neq 2c_3/3$ is available, and in this case, validity of (7′) for stage 3 only is reduced to $p_3 = 2$. For this type of method, the requirement for (7′′) to satisfy the order conditions is replaced by the cancellation of certain coefficients. Hence, in this case, it is convenient to specify the elements of the SOV by the satisfaction of (7′) only.

For methods of the type displayed in Tableau 12, only eight stages are needed if the fifth order method is propagated. This design was modified independently by Dormand et al. [10], Calvo et al. [5], and Verner [35] to allow the propagation of the sixth order approximation in the initial eight stages such as that of Tableau 15. Recently, the last of these approaches was extended by Verner and Sharp [39] to yield such pairs of order $p \geq 6$ with p arbitrary.

Tableau 15: A FSAL RK(9*, (5)6) pair with DSO=3

0										6
$\frac{1}{9}$	$\frac{1}{9}$									1
$\frac{1}{6}$	$\frac{1}{24}$	$\frac{1}{8}$								2
$\frac{1}{4}$	$\frac{1}{16}$	0	$\frac{3}{16}$							3
$\frac{5}{8}$	$\frac{5}{8}$	0	$-\frac{75}{32}$	$\frac{75}{32}$						3
$\frac{2}{3}$	$\frac{374}{1539}$	0	$-\frac{44}{57}$	$\frac{4880}{4617}$	$\frac{640}{4617}$					3
$\frac{7}{8}$	$-\frac{30023}{14592}$	0	$\frac{10353}{1216}$	$-\frac{35035}{5472}$	$-\frac{70}{171}$	$\frac{315}{256}$				3
1	$\frac{70169}{18620}$	0	$-\frac{1914}{133}$	$\frac{38592}{3325}$	$\frac{1392}{665}$	$-\frac{243}{100}$	$\frac{432}{1225}$			3
$\mathbf{b}^6$	$\frac{53}{700}$	0	0	$\frac{1264}{3375}$	$\frac{128}{675}$	$\frac{81}{500}$	$\frac{128}{875}$	$\frac{7}{135}$		6
$\mathbf{b}^5$	$\frac{137}{2100}$	0	0	$\frac{32}{75}$	$-\frac{64}{75}$	$\frac{27}{20}$	$-\frac{64}{525}$	0	$\frac{2}{15}$	5

Another kind of Runge-Kutta method has been proposed by Owren and Zennaro – continuous Runge-Kutta methods are designed specifically to provide an approximation at all points of an interval, rather than just for a discrete set. These methods have error estimators inherent in their design. Those authors have found eight-stage methods of order 5 [21,22].More recently, Santo [26] has shown that at least eleven stages are needed for continuous methods of order 6. Such methods include explicit Runge-Kutta methods with appended interpolants of the same order as a special case. A variety of interpolants of orders $p \leq 6$ have appeared in the literature. The techniques used by Verner [37] yield eleven-stage methods of order 6, and 15-stage methods of order 7, for example. Thus, there may be as much as a 50% additional cost over conventional pairs to obtain continuous approximations.

In addition to this construction of a variety of methods, there have been some attempts to identify explicit connections between different types of pairs. For example, it is known that each Fehlberg pair can be interpreted as the limit of a sequence of more general pairs [34]. Verner and Sharp [39] derived a new family of conventional eight-stage pairs of orders 5 and 6 by imposing an additional constraint on the nodes of nine-stage pairs with stage reuse.

5. A Classification Scheme

To summarize studies illustrated in preceeding sections, a scheme was developed for classifying pairs of methods. Through classifying the known pairs by similarities and differences in their structure, we can better identify the fundamental properties of methods which lead to their derivation. Better schemes may be possible, for example, by further study of the interaction of the order conditions.

For a convenient division into classes, there are several major types of error-estimating formulas:

I. Pairs with identical quadrature rules

II. Pairs with distinct quadrature rules using only internal stages

III. Pairs with reuse of the propagating stage (FSAL)

IV. Continuous methods

Methods of type III are further distinguished according to whether the lower- or higher-order approximation is reusable – with the latter denoted as type IIIX (to indicate that extrapolation is implemented).

Further, the dominant stage-order of a pair is used as a secondary classification. The variety of stage-order vectors for known pairs of design orders 6, 7 and 8 are surveyed in the following tables. As stated in §3, these pairs usually have $DSO = p - 4$ or $DSO = p - 3$.

The pairs included are consistent with the proposed classification scheme. However, for Hairer's seventeen-stage method of order 10, with a relaxed definition of stage-order a convenient value for the $DSO = 5 \equiv p - 5$, and this would preclude the method from this classification. A twelve-stage pair of this type has an ASOV=(8,1,2,3,3,4,4,4,3,1,4,4:8,7) which would suggest $DSO = 4 \equiv p - 4$, and difficulties with classifying an eight-stage pair of orders 5 and 6 have already been mentioned. Perhaps with further study an improved classification scheme may be contrived to resolve this deficiency.

Table 1: Stage-orders of some formulas of orders 5 and 6

Formula	Class	Stages	ASOV	DSO
Fehlberg	Ia	8	(6,1,2,2,2,3,2,2:6,5)	2
Hairer	Ib	8	(6,1,2,3,3,1,3,3:6,5)	3
Verner	IIa1	8	(6,1,2,2,2,2,2,2:6,5)	2
Prince-Dormand	IIa2	8	(6,1,2,2,2,2,2,2:6,5)	2
Butcher	IIIb	9*	(6,1,2,3,3,3,3,3,5:6)	3
Dormand et al. Calvo et al. Verner	IIIXb	9*	(6,1,2,3,3,3,3,3,6:5)	3
Verner	IIIXa	9*	(6,1,2,2,2,2,2,2,6:5)	2

* For a successful step, one stage is reusable in the next step.

Table 2: Stage-orders of some formulas of orders 6 and 7

Formula	Class	Stages	ASOV	DSO
Fehlberg	Ia	10	(7,1,2,3,3,3,3,4,3,3:7,6)	3
Verner	IIa1	10	(7,1,2,3,3,3,3,3,3,3:7,6)	3
Sharp-Verner	IIa2	10	(7,1,2,3,3,3,3,3,3,3:7,6)	3
Verner-Sharp	IIb	11	(7,1,2,3,3,4,4,4,4,4,4:7,6)	4
Verner-Sharp	IIIXb	12*	(7,1,2,3,3,4,4,4,4,4,4,7:6)	4

* For a successful step, one stage is reusable in the next step.

Table 3: Stage-orders of some formulas of orders 7 and 8

Formula	Class	Stages	ASOV	DSO
Fehlberg	Ia	13	(8,1,3,3,3,4,4,4,4,4,8,4,4:8,7)	4
Verner	IIa1	13	(8,1,2,3,3,4,4,4,4,4,4,4,4:8,7)	4
Prince-Dormand	IIa1	13	(8,1,2,3,3,4,4,4,4,4,4,4,4:8,7)	4
Verner-Sharp	IIb	14	(8,1,2,3,3,4,4,5,5,5,5,5,5,5;8,7)	5
Verner-Sharp	IIIXb	15*	(8,1,2,3,3,4,4,5,5,5,5,5,5,5,8:7)	5

* For a successful step, one stage is reusable in the next step.

A "box-score" of known pairs of each order $p \geq 6$ has a number of vacancies still remaining to be filled. Recent and current research has revealed several families which

Table 4: Known Runge-Kutta Pairs of orders 5 and 6

Type	Subtype:	DSO=2	DSO=3
I		Fehlberg[14]	Hairer[33]
II		Verner[32] Prince-Dormand[23] Verner[38]	Verner-Sharp[39]
III			Butcher[4]
IIIX		Verner[38]	Verner-Sharp[39]
IV			Zennaro-Santo[26]

Table 5: Known Runge-Kutta Pairs of orders 6 and 7

Type	Subtype:	DSO=3	DSO=4
I		Fehlberg[14]	
II		Verner[32] Sharp-Verner[34]	Verner-Sharp[39]
III			
IIIX			Verner-Sharp[39]
IV			

Table 6: Known Runge-Kutta Pairs of orders 7 and 8

Type	Subtype:	DSO=4	DSO=5
I		Fehlberg[14]	
II		Verner[32] Prince-Dormand[23]	Verner-Sharp[39]
III			
IIIX			Verner-Sharp[39]
IV			

are expected to contain some efficient algorithms [38,39]. For those vacancies which still remain, there may exist no appropriate pairs. However, each attempt made to construct pairs of a promising design indicated by this scheme has been successful. Once selected, each case was resolved by studying known pairs of similar type, and pursuing a formulation that had the potential of characterizing a pair of the proposed design. Further, each successful derivation used the basic formulation outlined in earlier sections.

We conclude this section with an example of a pair of type IIIXa. This family is not yet completely characterized, but a subset exists for which $c_3 = 1$ and nodes c_4, c_5, c_6 are constrained by

$$
\begin{aligned}
(14) \qquad & -171c_4^2c_5^2 + 255c_4^4c_5 - 810c_5^2c_4^4 + 12c_4^4 - 15c_4c_5^3 + 315c_4^2c_5^3 + 6c_6c_5^2 + 19c_4^2c_5 \\
& -229c_4^3c_5 - 3c_4c_6 - 3c_5c_6 + c_5^2 - 9c_4c_5^2 - c_4c_5 + 25c_4^2 - 41c_4^3 + 750c_5^2c_4^4c_6 \\
& +895c_5^2c_4^3 - 525c_5^2c_4^3c_6 - 120c_4^4c_6 - 87c_5^2c_4c_6 + 900c_4^4c_5^3 - 1110c_4^3c_5^3 \\
& -225c_4^3c_5c_6 + 270c_4^2c_5^2c_6 + 198c_4^3c_6 - 63c_4^2c_6 + 6c_5c_4^2c_6 + 48c_5c_4c_6 = 0
\end{aligned}
$$

which is linear in c_6. A particular pair of this type follows.

Tableau 16: A FSAL RK(9*, (5)6) pair with DSO=2

0										$\mid 6$
$\frac{1}{3}$	$\frac{1}{3}$									$\mid 1$
1	$-\frac{1}{2}$	$\frac{3}{2}$								$\mid 2$
$\frac{2}{5}$	$-\frac{4}{125}$	$\frac{66}{125}$	$-\frac{12}{125}$							$\mid 2$
$\frac{2}{3}$	$-\frac{22}{405}$	$\frac{22}{45}$	$-\frac{68}{1215}$	$\frac{70}{243}$						$\mid 2$
$\frac{163}{225}$	$\frac{152731}{1265625}$	$-\frac{34067}{3796875}$	$\frac{1543121}{34171875}$	$\frac{1296991}{2187000}$	$-\frac{154687}{6075000}$					$\mid 2$
$\frac{7}{8}$	$\frac{6554196313}{5848596480}$	$-\frac{6699}{2560}$	$\frac{7737793}{13455360}$	$\frac{5493818365}{3143172096}$	$\frac{58204125}{62193664}$	$-\frac{82110459375}{92505300992}$				$\mid 2$
1	$\frac{7626226}{3816645}$	$-\frac{5313}{1115}$	$\frac{9809}{10035}$	$\frac{59474065}{22269672}$	$-\frac{52227}{115960}$	$\frac{9632823750}{9348199471}$	$-\frac{18538496}{40187945}$			$\mid 2$
$\mathbf{b}$	$\frac{1457}{13692}$	0	0	$\frac{19625}{22192}$	$-\frac{4023}{1040}$	$\frac{48694921875}{10396203896}$	$-\frac{598016}{540645}$	$\frac{223}{744}$		$\mid 6$
$\mathbf{b}^5$	$\frac{524399}{4577040}$	0	$-\frac{3751}{52650}$	$\frac{34794925}{46736352}$	$-\frac{261577}{135200}$	$\frac{4873921875}{2179849204}$	$-\frac{11736064}{45182475}$	0	$\frac{111}{650}$	$\mid 5$

6. Conclusions

A variety of formula pairs have been examined with a view to identifying common features of their structure. It might be expected that such study will lead to an improved understanding of such methods, and probably to new methods and new kinds of methods should they exist.

A scheme is proposed to classify types of formula pairs according to similarities among and differences between their structures. While the proposed scheme is not completely consistent, it may be expected to facilitate the analysis of properties of different *classes* of methods.

The analysis has a broader application. New classes of hybrid and general linear methods continue to appear in the literature. In such methods, the lowest stage-order is often greater than 1, but perhaps less than the corresponding dominant stage-order. Hence, a classification scheme of the proposed type will be different, but may facilitate the derivation of new formulas.

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