Order Barriers and Characterizations for Continuous Mono-Implicit Runge-Kutta Schemes

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Abstract. The mono-implicit Runge-Kutta (MIRK) schemes, a subset of the family of implicit Runge-Kutta (IRK) schemes, were originally proposed for the numerical solution of initial value ODE's more than fifteen years ago. During the last decade, there has been considerable investigation of the use of these schemes in the numerical solution of boundary value ODE problems, where their efficient implementation suggests that they may provide a worthwhile alternative to the widely used collocation schemes. In fact, recent work in this area has seen the development of some software packages for boundary value ODE's based on these schemes. Unfortunately, these schemes lead to algorithms which provide only a discrete solution approximation at a set of mesh points over the problem interval, while the collocation schemes provide a natural continuous solution approximation. The availability of a continuous solution is important not only to the user of the software but also within the code itself, for example, in estimation of errors, defect control, mesh selection, and the provision of initial solution estimates for new meshes. An approach for the construction of a continuous solution approximation based on the MIRK schemes is suggested by recent work in the area of continuous extensions for explicit Runge-Kutta schemes for initial value ODE's. In this paper, we describe our work in the investigation of continuous versions of the MIRK schemes: (i) we give some lower bounds relating the stage order to the minimal number of stages for general IRK schemes, (ii) we establish lower bounds on the number of stages needed to derive continuous MIRK schemes of orders 1 through 6, (iii) we provide characterizations of such schemes having a minimal number of stages for each of these orders.

Keywords: Runge-Kutta methods, boundary value ODE's, continuous extensions

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1. Introduction

An implicit Runge-Kutta (IRK) scheme (see, for example, [Butcher 1987]), can be used to compute an approximation to the solution of the initial value problem (IVP)

$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0, \tag{1.1}$$

where $y(x) \in R^m$, $f : R \times R^m \rightarrow R^m$, and $y_0 \in R^m$ is a given initial condition. The IRK scheme is used in a stepwise fashion to proceed from the initial conditions through a sequence of points, x_i, and solution approximations, y_i, to the desired termination point. During the ith step, we obtain an approximation, y_{i+1}, to the true solution, $y(x)$, evaluated at the point $x_{i+1} = x_i + h_i$, of the form,

$$y_{i+1} = y_i + h_i \sum_{r=1}^{s} b_r K_r, \tag{1.2}$$

where

$$K_r = f(x_i + c_r h_i, y_i + h_i \sum_{j=1}^{s} a_{rj} K_j), \qquad r = 1, \ldots, s, \tag{1.3}$$

where $c_r = \sum_{j=1}^{s} a_{rj}$. These schemes are sometimes given in the form of a tableau containing their coefficients, which, for the above scheme, would have the following form

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

The above tableau is sometimes written in the more compact form

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

where $c = Ae$, $c = (c_1, c_2, \ldots, c_s)^T$, $b = (b_1, b_2, \ldots, b_s)^T$, A is the s by s matrix whose (i, j)-th component is a_{ij}, and e is the vector of 1's of length s. Note that in (1.2) above, each stage is defined implicitly in terms of itself and the other stages. Hence in order to obtain approximate values for the stages it is necessary to solve a system of, in general, non-linear equations. This must usually be done using some form of modified Newton iteration, which makes the calculation of the stages a somewhat computationally expensive process.

A number of interesting subclasses of the IRK schemes have been identified and investigated in the literature. These schemes represent attempts to trade-off the higher accuracy of the IRK schemes for schemes which can be implemented more efficiently. Examples of such schemes are singly-implicit Runge-Kutta schemes [Burrage 1978], diagonally implicit Runge-Kutta schemes [Nørsett 1974], and the mono-implicit Runge-Kutta (MIRK) schemes [Cash and Singhal 1982a] (also known as implicit endpoint quadrature formulas [Van Bokhoven 1980]).

In this paper, we will primarily focus on the class of MIRK schemes. These scheme are defined with a slightly alternative representation to that of the IRK schemes, which involves the introduction of s new parameters, $v_r, r = 1, \ldots, s$, that allow for explicit dependence on y_{i+1} in the definition of the stages of the scheme. The standard form of this class is

$$y_{i+1} = y_i + h_i \sum_{r=1}^{s} b_r K_r, \tag{1.4}$$

where

$$K_r = f(x_i + c_r h_i, (1 - v_r)y_i + v_r y_{i+1} + h_i \sum_{j=1}^{r-1} x_{rj} K_j), \qquad r = 1, \ldots, s, \tag{1.5}$$

where $c_r = v_r + \sum_{j=1}^{s} x_{rj}$. They are usually represented by a modified tableau; the above method would have the tableau,

$$\begin{array}{c|c|cccccc}
c_1 & v_1 & 0 & 0 & \ldots & 0 & 0 \\
c_2 & v_2 & x_{21} & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
c_{s-1} & v_{s-1} & x_{s-1,1} & x_{s-1,2} & \ldots & 0 & 0 \\
c_s & v_s & x_{s,1} & x_{s,2} & \ldots & x_{s,s-1} & 0 \\
\hline
 & & b_1 & b_2 & \ldots & b_{s-1} & b_s
\end{array}$$

which is sometimes written in the more compact form

$$\begin{array}{c|c|c}
c & v & X \\
\hline
 & & b^T
\end{array}$$

where $v = (v_1, v_2, \ldots, v_s)^T$, $c = v + Xe$, and X is strictly lower triangular. These schemes are interesting because they are implicit only in y_{i+1}; this leads to a more efficient implementation than is possible for the fully implicit IRK schemes [Van Bokhoven 1980].

The use of IRK schemes for the solution of boundary value ODE problems (BVP) has been well-known for some time [Weiss 1974]. In this paper, we assume that the boundary value ODE's are expressed in the general form,

$$y'(x) = f(x, y(x)), \qquad x \in [a, b], \tag{1.6}$$

where $y \in R^m$ and $f : R \times R^m \rightarrow R^m$ with boundary conditions,

$$g(y(a), y(b)) = \underline{0}, \tag{1.7}$$

where $g : R^m \times R^m \rightarrow R^m$. The main step in a Runge-Kutta based algorithm for the numerical solution of a boundary value ODE is the solution of a discrete system, $\Phi(Y) = 0$, where Y is a vector whose i-th component, y_i, is an approximation to the exact solution evaluated at the i-th point of an $N + 1$ point mesh which subdivides the problem interval. $\Phi(Y)$ can be expressed in a component-wise form with one component of size m for the boundary conditions, g, and N components, each of size m, ϕ_i, $i = 0, \ldots, N - 1$, where ϕ_i is defined by an IRK scheme. We have,

$$\phi_i = y_{i+1} - y_i - h_i \sum_{r=1}^{s} b_r K_r, \tag{1.8}$$

with the stages, K_r, defined as in (1.3). As in the IVP case, when all the a_{rj} coefficients are non-zero, the stages are defined implicitly and in order to compute them we will, in general, have to solve a system of nonlinear equations.

The implicit Runge-Kutta formulas include the collocation formulas which have been a popular approach for the numerical solution of boundary value ODE's. The collocation formulas based on Gauss-point rules have been implemented in the widely used code, COLSYS [Ascher, Christiansen, and Russell, 1981], and its successor, COLNEW [Bader and Ascher 1987]. However, compared to the situation for IVP's, there has been relatively little work done in the investigation of efficient subclasses of the IRK schemes for boundary value ODE's. Most of the subclasses presented to date have been based on the class of MIRK schemes. A single formula from this subclass of schemes was first suggested for use in the numerical solution of boundary value ODE's in [Cash and Moore 1980]. This result was generalized in [Cash and Singhal 1982b], where a symmetric subclass of the MIRK schemes was presented. The use of these schemes within an iterated deferred correction scheme for the numerical solution of boundary value problems has been described in [Cash 1986,1988], and [Cash and Wright 1989]. This work has led to the development of a code called HAGRON which has been shown to compare favorably with COLSYS and D02GAF, a code from the NAG library based on PASVA3 [Lentini and Pereyra 1977]. The entire class of MIRK schemes has been considered for use in the numerical solution of boundary value ODE's in [Gupta 1985] and [Enright and Muir 1986].

When a MIRK scheme is used within the algorithm outlined above for the solution of boundary value ODE's, it defines equations having the same form as in (1.8) but the corresponding stages are of the mono-implicit type and have the form (1.5). However, in the BVP context, since approximations to both y_i and y_{i+1} are available from the current Newton iterate, the stages of the MIRK scheme can be computed explicitly, and thus very efficiently. These improvements in efficiency are not gained, however, by giving up good stability as is the case for explicit Runge-Kutta schemes. There are many instances of MIRK schemes which are symmetric and A-stable, two important properties for discretization schemes used in the numerical solution of boundary value ODE's.

An important advantage of the collocation formulas is that a continuous approximation to the solution over the entire problem interval is naturally obtained. This can be very useful when the user requires solution information at off mesh points, but the continuous solution approximation can also be useful to the code itself, for example, for error estimation, defect control, provision of initial estimates for Newton iterates, or mesh refinement and redistribution. Unlike the collocation formulas, many other schemes do not have an associated natural continuous approximation to the solution. Examples of codes based on such schemes are D02GAF, mentioned earlier, some codes based on special one-sided Runge-Kutta schemes [Kreiss, Nichols, and Brown 1986], [Brown and Lorenz 1987], and the HAGRON code, mentioned above.

In the area of initial value ODE problems, the idea of extending the discrete solution approximation to get a continuous solution has received considerable attention over the last few years. A number of authors have demonstrated the possibility of generating inexpensive interpolants for explicit Runge-Kutta formulas which are not of the collocation type, in the context of the numerical solution of initial value problems; see, for example, [Enright et al. 1986], [Gladwell et al. 1987] and references within for some of the earlier work. These interpolants are obtained for Runge-Kutta formula pairs, by constructing extra stages within the current step, thus preserving the one-step nature of the formula. The most recent work on these continuous explicit Runge-Kutta schemes has been described in [Owren and Zennaro 1991a, 1991b] and [Verner 1990].

[Nørsett and Wanner 1981] considered perturbed collocation schemes and proved that any non-confluent Runge-Kutta scheme is equivalent to a generalized type of collocation with a polynomial of degree s. The usefulness of the perturbed collocation polynomial as a continuous extension of the Runge-Kutta scheme has been limited by some undesirable properties of these approximations. For instance, as the authors point out, the higher derivatives of the approximation may become unbounded as the step size tends to zero. A slightly different approach is taken in [Zennaro 1986] where it is proved that any Runge-Kutta scheme of order p possesses *natural continuous extensions* (NCE) of some degree $d \leq p$. These continuous approximations have uniform order d and satisfy certain orthogonality conditions which make them particularly useful for solving ODE's which contain forcing terms. Collocation schemes and, in fact, also a subclass of the perturbed collocation schemes, are themselves NCE's. In [Zennaro 1988] the related class of projection schemes is considered. Introducing a linear projector $Q_d : C^0[x_i, x_i + h_i] \to \Pi_{d-1}$, where Π_{d-1} is the set of polynomials of degree $\leq d-1$, he considers the polynomial, $u(x)$, defined by $u'(x) = Q_d f(x, u(x))$. Again it is interesting to observe that the collocation schemes turn out to be a subclass.

The basic form of a continuous Runge-Kutta (CRK) scheme on the ith step is a polynomial in θ of the form

$$u(x_i + \theta h_i) = y_i + h_i \sum_{r=1}^{s} b_r(\theta) K_r, \tag{1.9}$$

where

$$K_r = f(x_i + c_r h_i, y_i + h_i \sum_{j=1}^{s} a_{rj} K_j), \quad r = 1, \ldots, s. \tag{1.10}$$

Observe that the stage values K_r, $r = 1, \ldots, s$, are the same as for the discrete Runge-Kutta scheme, (1.3). We assume that $b_r(\theta), i = 1, \ldots, s$, are weight polynomials of some maximum degree d. It is easy to see that in order to obtain continuity of the global piecewise continuous approximation furnished by a CRK scheme, one must require that $b_r(0) = 0$ for all the weight polynomials, see e.g. [Verner 1990]. We will tacitly assume this property for the schemes we consider. Notice also that any CRK scheme has an underlying discrete scheme defined by the coefficient matrix A and with discrete weights $b_r = b_r(1), r = 1, \ldots, s$.

For boundary value ODE's, the extension of discrete solution approximations to get continuous ones has received substantially less attention. [Pruess 1986] is concerned with the development of interpolants for collocation schemes for boundary value problems where the information required to construct a continuous approximation is not available and one has only solution approximations at the mesh points.

In this paper, we investigate continuous versions of the MIRK schemes, (which we will refer to as CMIRK schemes) with the idea of providing continuous solutions for boundary value ODE's. The continuous MIRK schemes have the form as above in (1.9) except that the corresponding stages will be of mono-implicit type, (1.5). This paper is organized as follows. In section 2, we present some theoretical results concerned with continuous extensions for general IRK schemes. In section 3, these results are applied to derive order barriers for continuous MIRK schemes of orders 1 through 6. Characterizations of families of continuous MIRK schemes of orders 1 through 6 are given in section 4. We conclude in section 5, with a summary of our results and a discussion of future work.

2. Some General Theory for Continuous Runge-Kutta Schemes

In this section we will develop some general tools for the derivation and order barrier analysis of CRK schemes, (1.9),(1.10) following the ideas of [Owren and Zennaro 1991a], [Owren and Zennaro 1991b]. Without loss of generality we shall henceforth consider continuous approximations to $y(x)$ on the first step interval (from x_0 to x_1), and we shall omit step indices where it does not cause ambiguity. We define the *uniform order* of a CRK scheme (1.9), (1.10), as the greatest integer p for which

$$\max_{0 \leq \theta \leq 1} |y(x_0 + \theta h) - u(x_0 + \theta h)| = O(h^{p+1}), \tag{2.1}$$

where $u(x_0) = y(x_0)$ and $|\cdot|$ is any norm on R^m.

In the following we will use the theory of trees and order conditions introduced in [Butcher 1963, 1964] without further citations. We recommend the excellent text [Butcher 1987] for an account of this material. The adaptations of this theory to continuous schemes involve generalizations of the ideas of [Owren and

Zennaro 1991a]. In order to clarify our notation we will briefly review some of the main results from that paper. It was remarked in [Zennaro 1986] that the maximum degree d of the weight polynomials must be at least p for (2.1) to be satisfied, and that $d > p$ can lead to unbounded derivatives of $u(x)$ as h tends to zero, hence we will always assume that $d = p$. This requirement and (2.1) cause the CRK scheme, (1.9),(1.10), to be a natural continuous extension of the underlying discrete scheme, as defined in [Zennaro 1986]. Let N_p be the total number of rooted trees of order at most p and let $t_1, \ldots, t_{N_p}$ be any ordering of these trees such that $\rho(t_i) > \rho(t_j)$ only if $i > j$ where $\rho(t_k)$ is the order of t_k. Following [Butcher 1987, p.163] we introduce the elementary weight $\phi_{ij} := \phi_j(t_i)$ for each tree t_i and stage j, and we let $\gamma(t_i)$ be the *density* of t_i. Then (2.1) is satisfied if and only if

$$\sum_{j=1}^{s} \phi_{ij} b_j(\theta) = \frac{\theta^{\rho(t_i)}}{\gamma(t_i)}, \; i = 1, \ldots, N_p.$$

Since $\rho(t_i) \geq 1$ for all t_i and since $b_i(0) = 0$ for all the weight polynomials, we may write

$$b_i(\theta) = \sum_{j=1}^{p} b_{ij}\theta^j \qquad \text{and} \qquad \frac{\theta^{\rho(t_i)}}{\gamma(t_i)} = \sum_{l=1}^{p} q_{il}\theta^l. \tag{2.2}$$

Thus, by defining the $N_p \times s$ matrix $\Phi := ((\phi_{ij}))$, the $s \times p$ matrix $B := ((b_{ij}))$ and the $N_p \times p$ matrix $Q := ((q_{il}))$ we arrive at the matrix equation

$$\Phi B = Q. \tag{2.3}$$

From classical order theory for Runge-Kutta schemes we know that Φ only depends on the $s \times s$ matrix A and from (2.2) we see that Q is a constant matrix, in fact it has the simple form $q_{il} = \gamma(t_i)^{-1}\delta_{\rho(t_i)l}$. Clearly the columns of Q must be linearly independent, so $\operatorname{rank}(Q) = p$. It will be convenient to view the matrix Φ as the image of a nonlinear operator whose domain is the union over all positive s of the sets of all $s \times s$ matrices A and we denote this operator by $F_p(A)$. We will also need another operator with the same domain, namely $G_p(A) := (F_p(A)|Q)$, i.e. the matrix Φ augmented by the columns of Q. We summarize some properties of these matrices.

Lemma 2.1

$$\operatorname{rank}(G_p(A)) \geq p, \tag{2.4}$$

$$\operatorname{rank}(G_{p+1}(A)) \geq \operatorname{rank}(G_p(A)) + 1, \tag{2.5}$$

$$\operatorname{rank}(F_p(A)) \leq s, \tag{2.6}$$

$$\operatorname{rank}(F_p(A)) \geq p \text{ if at least } p \text{ of the } c_i\text{'s are distinct.} \tag{2.7}$$

Proof. (2.6) is obvious. (2.4) and (2.5) follow easily by considering the last p columns of $G_p(A)$. We see that (2.7) holds when at least p of the c_i's are distinct because the rows of $F_p(A)$ corresponding to the trees τ and $[\tau^k]$, $1 \leq k \leq p-1$ define a vandermonde system, see e.g. [Verner 1990]. ∎

It is well-known that the rows of $F_p(A)$ can be generated recursively by forming componentwise products between previously generated rows, or by multiplying a previously generated row by the matrix A. We will sometimes find it convenient to write $zw = (z_1w_1, \ldots, z_sw_s)^T$ where $z = (z_1, \ldots, z_s)^T$ and $w = (w_1, \ldots, w_s)^T$. Similarly we write $z^k = (z_1^k, \ldots, z_s^k)^T$. Finally we define C to be the diagonal matrix with $c_1, \ldots, c_s$ on the diagonal. The following result is an obvious generalization of a result in [Owren and Zennaro 1991a].

Proposition 2.2 An $s \times s$ matrix A defines the coupling coefficients of an s stage CRK scheme of order p if and only if $\operatorname{rank}(F_p(A)) = \operatorname{rank}(G_p(A))$.

We are seeking CRK schemes that have the minimal number of stages. To this end, we generalize another result from [Owren and Zennaro 1991a].

Theorem 2.3 Let A be an $s \times s$ matrix such that rank$(F_p(A))$ =rank$(G_p(A)) = \rho < s$. Then there exists a $\rho \times \rho$ matrix A^* such that rank$(F_p(A^*))$ =rank$(G_p(A^*)) = \rho$.

Proof. The proof is based on the same ideas as those of Theorem 2.4 in [Owren and Zennaro 1991a]. It is sufficient to argue that there exists an $(s-1)\times(s-1)$ matrix A' satisfying rank$(F_p(A'))$ =rank$(G_p(A')) = \rho$. This argument may be applied $s-\rho$ times in order to prove the theorem. By assumption, (at least) one, say the kth column of $\Phi := F_p(A)$ depends linearly on the others, i.e.

$$(\phi_{1k}, \ldots, \phi_{N_p k})^T = \sum_{j\neq k} \lambda_j (\phi_{1j}, \ldots, \phi_{N_p j})^T, \tag{2.8}$$

for some $\lambda_j \in R$. We define the $s \times s$ matrix A'' as follows:

$$a''_{kj} := 0, \ \forall j, \quad a''_{ik} := 0, \ \forall i,$$

$$a''_{ij} := a_{ij} + \lambda_j a_{ik}, \ i \neq k, \ j \neq k.$$

It follows readily that the kth column of $\Phi'' := F_p(A'')$ equals $(1, 0, \ldots, 0)^T$. Next we will prove that the remaining columns of Φ'' equal the corresponding columns of Φ. We use induction on the row index, i, of these matrices and exploit the fact that the conditions are numbered increasingly in terms of their order. The result holds for $i = 1$ since the first row of $F_p(A)$ equals $(1, \ldots, 1)$ for any A. Now we assume that the result holds for any $i \leq n-1$ and prove it for $i = n$. The nth row corresponds to a tree t_n of order at least 2 which either has the form $[t_{n'}]$ where $\rho(t_{n'}) = \rho(t_n) - 1$, or it has the form $t_n = [t_{\nu_1}, \ldots, t_{\nu_r}]$ for $r(\geq 2)$ trees t_{ν_j}. In the latter case, $1 \leq \rho(t_{\nu_j}) \leq \rho(t_n) - 2$ and $\rho(t_n) = 1 + \sum_{j=1}^{r} \rho(t_{\nu_j})$. In the former case we get for $1 \leq j \leq s$ using the induction hypothesis

$$\phi''_{nj} = \sum_{l=1}^{s} a''_{jl}\phi_{n'l} = \sum_{l\neq k} a_{jl}\phi_{n'l} + a_{jk} \sum_{l\neq k} \lambda_l \phi_{n'l}.$$

Using (2.8) for the last sum we get

$$\phi''_{nj} = \sum_{l\neq k} a_{jl}\phi_{n'l} + a_{jk}\phi_{n'k} = \sum_{l=1}^{s} a_{jl}\phi_{n'l} = \phi_{nj}, \ j = 1, \ldots, s.$$

The latter case follows readily by induction since, with $t_{n_j} = [t_{\nu_j}]$, $n_j < n$ for all j and

$$\phi''_{nj} = \prod_{l=1}^{r} \phi''_{n_l j} = \prod_{l=1}^{r} \phi_{n_l j} = \phi_{nj}.$$

Thus we have established that all but the kth column Φ'' are equal to those of Φ. Furthermore, since the first column of Q is equal to $(1, 0, \ldots, 0)^T = (\phi''_{1k}, \ldots, \phi''_{N_p k})^T$, it follows, by virtue of (2.8), that the equation

$$\Phi'' B = Q$$

has a solution with the kth row of B equal to zero, corresponding to $b_k(\theta) \equiv 0$. So the kth stage of the scheme defined by A'' is of no use. Therefore, the kth row and column of A'' can be deleted in order to obtain the $(s-1) \times (s-1)$ matrix A' which must satisfy rank$(F_p(A'))$ =rank$(G_p(A')) = \rho$. This completes the proof. ∎

The above theorem allows us to restrict our attention to CRK schemes with coupling coefficients A such that $F_p(A)$ has linearly independent columns, since we know that schemes with the minimal number of stages must satisfy this property. It is easy to see that if two rows of the matrix A are identical, then they generate two identical columns of $F_p(A)$. Hence we have

Corollary 2.4 Assume that the $s \times s$ matrix A defines a CRK scheme of order p with the minimal number of stages. Then it cannot have two identical rows.

For our further discussion, we need a definition introduced in [Butcher 1964].

Definition 2.5 Consider the conditions

$$k \sum_{j=1}^{s} a_{ij} c_j^{k-1} = c_i^k, \quad 1 \le k \le \xi. \tag{2.9}$$

If an $s \times s$ matrix A is such that (2.9) holds for $1 \le i \le s$, we say that A satisfies $C(\xi)$. If (2.9) holds for $i = l$ we say that stage l of the corresponding scheme satisfies $C(\xi)$. (If the matrix, A, is the matrix of coupling coefficients of an IRK scheme it usual to also say that the IRK scheme itself satisfies the $C(\xi)$ conditions).

It is well known from classical theory for Runge-Kutta schemes that when $C(\xi)$, $\xi > 1$, is imposed on A, the complexity of the system of order conditions is significantly reduced. This is indeed the case also for CRK schemes. To quantify this, we will first present an enumeration result for a subset of the rooted trees. We will say that a rooted tree contains a k-leaf if it has a node, different from the root, which has at most $k-1$ children, all of which must be leaves.

Theorem 2.6 Let α_j, $j \ge 1$, be the number of rooted trees of order j which do not contain any k-leaves. Then $\alpha_1, \alpha_2, \ldots$ satisfy the relation

$$\alpha_1 + \alpha_2 x + \alpha_3 x^2 + \ldots = (1-x)^{-1} \prod_{n=k+1}^{\infty} (1-x^n)^{-\alpha_n}.$$

Proof. Similar to that of [Butcher 1987, Thm 145A, p89].

Corollary 2.7 $\alpha_j = 2^q$ where $q = \max\{0, j-k-1\}$ for $1 \le j \le 2k+2$.

These enumeration results may be used to provide upper bounds for the number of stages needed to construct a CRK scheme of a given order. We have

Theorem 2.8 Assume that an $s \times s$ matrix, A satisfies $C(\xi)$ for some $\xi \ge 1$. Let α_j be the number of rooted trees of order j without ξ-leaves and for each p define $r_p = \sum_{j=1}^{p} \alpha_j$. Then

$$\operatorname{rank}(G_p(A)) \le r_p.$$

Proof. It is clear, see e.g. [Butcher 1987, p.194, 214], that when A satisfies $C(\xi)$, any row of $G_p(A)$ that originates from a tree t_i containing a ξ-leaf, will be proportional to another row of $G_p(A)$ which originates from a tree t_j that does not contain a ξ-leaf where $\rho(t_i) = \rho(t_j)$. ∎

Theorem 2.9 The $s \times s$ matrix A defines the stages of an s-stage CRK scheme of order s if and only if it satisfies $C(s-1)$ and the numbers $c_i = \sum_{j=1}^{s} a_{ij}$ are all distinct.

Proof. Assume $C(s-1)$ holds for distinct c_i's. Then according to Corollary 2.7, Theorem 2.8 and (2.4) we get $\text{rank}(G_s(A)) = s$. Since the c_i's are distinct, we have $\text{rank}(F_s(A)) = s$ by (2.7) and (2.6), thus by Proposition 2.2, A defines the desired scheme. Conversely, assume that A represents a scheme of order s. Then, similarly we must have $\text{rank}(G_s(A)) = s$. Thus, (2.4) and (2.5) imply that row i and j must be proportional if $\rho(t_i) = \rho(t_j)$. In particular this means that the pairs of rows originating from $[\tau^l]$ and $[[\tau^{l-1}]]$ must be proportional for $2 \le l \le s-1$. But this means that $c^l = lAc^{l-1}$ for $1 \le l \le s-1$ which is exactly the conditions $C(s-1)$. Furthermore, it follows that the row space of $F_s(A)$ is spanned by the vectors c^k, $0 \le k \le s-1$, and hence $\text{rank}(F_s(A)) = s$ if and only if the c_i's are distinct. ∎

For an $s \times s$ matrix A we introduce the following equivalence relation on the set of indices $\{1, \dots, s\}$:

$$i \equiv j \quad \text{if and only if } c_i = c_j.$$

Let s^* be the number of equivalence classes, which we label $S_1, \dots, S_{s^*}$.

The theorem above shows that the CRK schemes of order p that have the minimal number of stages are the ones which satisfy $C(p-1)$. In fact, these schemes can be recognized as perturbed collocation (PECO) schemes where the collocation polynomial is identical to the continuous approximation $u(x)$. From [Nørsett and Wanner 1981] we have the perturbation operator, $P : \Pi_s \to \Pi_s$, defined by

$$Pu(x) := u(x) + \sum_{j=1}^{s} N_j(\theta) u^{(j)}(x_0) h^j, \quad 0 \le \theta = \frac{x - x_0}{h} \le 1,$$

where the $N_j(\theta)$'s are polynomials of degree $\le s$. Then the PECO scheme is

$$\begin{aligned} u(x_0) &= y_0, \\ u'(x_0 + c_r h) &= f(x_0 + c_r h, Pu(x_0 + c_r h)), \quad r = 1, \dots, s, \\ y_1 &= u(x_0 + h), \end{aligned}$$

where the c_r's are distinct. We have the following relationship between the schemes of Theorem 2.9 and PECO schemes.

Theorem 2.10 A CRK scheme of order p with p stages is equivalent to a PECO scheme with $N_1(\theta) = \cdots = N_{p-1}(\theta) \equiv 0$ and $N_p(\theta) \in \Pi_{p-1}$, a polynomial of degree $p-1$, such that

$$N_p(c_r) = -\frac{1}{p!}\left(c_r^p - p \sum_{j=1}^{p} a_{rj} c_j^{p-1}\right), \quad r = 1, \dots, p.$$

Prior to proving this theorem, we consider the following lemma.

Lemma 2.11 Let A define a CRK scheme of order p with weight polynomials $b_j(\theta)$, $j = 1, \dots, s$. Assume that exactly p of these polynomials, $b_{i_1}(\theta), \dots, b_{i_p}(\theta)$, $i_r \in \{1, \dots, s\}, r = 1, \dots, p$, are non-zero. Then

$$\begin{aligned} K_{i_r} &= u'(x_0 + c_{i_r} h), \quad r = 1, \dots, p, \\ b'_{i_r}(\theta) &= L_{i_r}(\theta), \quad r = 1, \dots, p, \end{aligned}$$

where $L_{i_r}(\theta)$ is the i_rth Lagrange interpolation function with respect to the points $\{c_{i_1}, \dots, c_{i_p}\}$.

Proof. Such CRK schemes must in particular satisfy the quadrature conditions

$$\sum_{r=1}^{p} b_{i_r}(\theta) c_{i_r}^{k-1} = \frac{\theta^k}{k}, \quad k = 1, \dots, p.$$

Differentiating we get

$$\sum_{r=1}^{p} b'_{i_r}(\theta) c_{i_r}^{k-1} = \theta^{k-1}, \quad k = 1, \ldots, p,$$

thus the polynomials $b'_{i_r}(\theta),\ r = 1, \ldots, p$ form a basis for Π_{p-1}. In fact, for any $p(\theta) \in \Pi_{p-1}$ we have

$$p(\theta) = \sum_{r=1}^{p} p(c_{i_r}) b'_{i_r}(\theta),$$

from which it follows that that $b'_{i_r}(\theta) = L_{i_r}(\theta),\ r = 1, \ldots, p$. Since $u'(x_0 + \theta h) = \sum b'_{i_r}(\theta) K_{i_r}$, we have $u'(x_0 + c_{i_r} h) = K_{i_r},\ r = 1, \ldots, p$. ∎

We now employ this lemma in the proof of Theorem 2.10.

Proof of Theorem 2.10. Let $w := (N_p(c_1), \ldots, N_p(c_p))^T$ and let b_p be the pth column of the weight matrix B. Let M be the $p \times p$ matrix whose (i,j)th element is $b_j(c_i)$. We argue that for the CRK schemes of Theorem 2.9 we have $A = M + (p!) w b_p^T$. To show this, we multiply $M + (p!) w b_p^T$ with the $p \times p$ matrix V whose columns are $c^0, c^1, \ldots, c^{p-1}$. The quadrature conditions imply $M c^{k-1} = c^k / k,\ k = 1, \ldots, p$. By (2.3) we get $b_p^T c^{k-1} = \delta_{pk}/k$. Hence, for $k \le p-1$ we get $(M + (p!) w b_p^T) c^{k-1} = c^k / k = A c^{k-1}$ since $C(p-1)$ holds for A while $(M + (p!) w b_p^T) c^{p-1} = c^p / p + (p!) w / p = A c^{p-1}$. Thus $AV = (M + (p!) w b_p^T) V$ which implies $A = M + (p!) w b_p^T$ since V is non-singular (because the c_i's are distinct). Now we apply Lemma 2.11 with $s = p$ to obtain

$$\begin{aligned} u'(x_0 + c_r h) = K_r &= f(x_0 + c_r h, y_0 + h \sum_{j=1}^{p} a_{rj} K_j) \\ &= f(x_0 + c_r h, y_0 + h \sum_{j=1}^{p} b_j(c_r) K_r + (p!) h \sum_{j=1}^{p} N_p(c_r) b_{jp} K_j),\ r = 1, \ldots, p. \end{aligned}$$

Since $u^{(p)}(x_0) h^p = (p!) h \sum_{j=1}^{p} b_{jp} K_j$ we get

$$u'(x_0 + c_r h) = f(x_0 + c_r h, u(x_0 + c_r h) + N_p(c_r) h^p u^{(p)}(x_0)),$$

and we have proved that our CRK scheme is indeed the PECO scheme above. ∎

In the following, we shall be concerned with schemes of order, say q, which fail to satisfy $C(q-1)$. Under such circumstances the following theorem provides a lower bound for the minimum number of stages needed to obtain a given order.

Theorem 2.12 For an $s \times s$ matrix A, let $k \ge 2$ be the largest integer such that $C(k-1)$ holds for A. Let $u_i = c_i^k - k \sum_{j=1}^{s} a_{ij} c_j^{k-1}$ for $1 \le i \le s$, and let e_i be the ith canonical unit vector. Then for any $q \ge k+1$,

$$\operatorname{rank}(G_q(A)) \ge q + 1. \tag{2.10}$$

Moreover, if $q > k+1$ and $\operatorname{rank}(G_q(A)) = \operatorname{rank}(F_q(A)) = q + 1$ then there exists $L \in \{1, \ldots, s^*\}$ such that

(i) $|S_L| = 2$ and $|S_i| = 1,\ i \ne L$.

(ii) $C(q-1)$ holds for all stages $i \notin S_L$, and there exist real numbers β_l such that

$$c_i^l - l \sum_{j=1}^{s} a_{ij} c_j^{l-1} = \beta_l u_i,\ i \in S_L,\ k+1 \le l \le q-1. \tag{2.11}$$

(iii) There exists $\lambda \in R$ such that

$$\sum_{i \in S_L} u_i (A - \lambda I) e_i = 0. \tag{2.12}$$

Proof. (2.10) is an obvious consequence of Theorem 2.9 since, by assumption, $C(q-1)$ is not satisfied. To prove the second part assume that $\text{rank}(F_q(A)) = \text{rank}(G_q(A)) = q+1$ for $q > k+1$. In view of (2.5) it is then necessary that $\text{rank}(G_{k+2}(A)) = k+3$. From Theorem (2.8) we deduce that there are at most two linearly independent conditions of order $k+1$ and four of order $k+2$. By (2.10) at least $k+2$ conditions of order at most $k+1$ are linearly dependent. To impose $\text{rank}(G_{k+2}(A)) = k+3$ we consider the conditions of order $k+2$, and we need to look at the conditions corresponding to the trees $[\tau^{l-1}], [[\tau^{l-2}]]$, $k+1 \le l \le q-1$. Introducing, $\mu_1, \mu_2, \beta_{k+1}, \ldots, \beta_{q-1} \in R$ we obtain the following conditions,

$$\mu_1(c^k - kAc^{k-1}) = c^{k+1} - kcAc^{k-1}, \tag{2.13}$$

$$\mu_2(c^k - kAc^{k-1}) = c^{k+1} - k(k+1)A^2c^{k-1}, \tag{2.14}$$

$$\beta_l(c^k - kAc^{k-1}) = c^l - lAc^{l-1}, \; k+1 \le l \le q-1. \tag{2.15}$$

Putting $u = (u_1, \ldots, u_s)^T$ we get from (2.13) that $Cu = \mu_1 u$, and since C is diagonal there must be an $L \in \{1, \ldots, s^*\}$ such that stage i satisfies $C(k)$ for $i \notin S_L$, i.e. $c^k - kAc^{k-1} = \sum_{i \in S_L} u_i e_i$. (ii) now follows readily from (2.15). Using this in (2.14) we get

$$\mu_2 \sum_{j \in S_L} u_j e_j = c^{k+1} - (k+1)A(c^k - \sum_{j \in S_L} u_j e_j) = \sum_{j \in S_L} \beta_{k+1} u_j e_j + (k+1) \sum_{j \in S_L} u_j A e_j,$$

hence

$$\sum_{j \in S_L} u_j (A - \lambda I) e_j = 0,$$

where $\lambda = (\mu_2 - \beta_{k+1})/(k+1)$. Finally, S_L must contain more than one element, since otherwise, we get with $j \in S_L$, $b_j(\theta) \equiv 0$ and $a_{ij} = 0$, $i \neq j$ such that the scheme would be reducible in the sense of [Dahlquist and Jeltsch 1979]. On the other hand, $s^* \ge q$, see e.g. [Zennaro 1986], hence (i) follows. ∎

An interesting question is whether there exist CRK schemes with coefficient matrix, A, satisfying the conditions (i)–(iii) in Theorem 2.12. Indeed it can be shown that, for instance, with $k = 2$ (only $C(1)$ satisfied) one can construct CRK schemes of order 4 having 5 stages. This can be done even with the CMIRK schemes, where the form of the A matrix is somewhat restricted.

3. Order barriers for CMIRK schemes

In this section we will derive the minimum number of stages CMN(p) needed to construct CMIRK schemes of orders p =1, ...,6. It is known from [Burrage, Chipman, and Muir 1991] that the largest integer k for which $C(k)$ can be satisfied for a CMIRK scheme is 3. We may therefore immediately conclude from Theorem 2.9 and (2.4) that CMN(p) = p for $1 \le p \le 4$. The same theorem in conjunction with Theorem 2.8 proves that CMN(5)=6. From these theorems we see that a 5th order CMIRK scheme with 6 stages can be constructed by imposing $C(3)$ on A. We shall see that this condition is also necessary. We have

Theorem 3.1 Let the $s \times s$-matrix A define a CMIRK scheme which does not satisfy $C(3)$. If $s = \text{rank}(G_q(A)) = \text{rank}(F_q(A))$ with $q \ge 5$ then $s \ge q+2$.

Proof. We prove that if $C(3)$ does not hold then the requirement $\text{rank}(G_q(A)) = q+1$ implies that either two rows of A are identical, which is impossible in view of Corollary 2.4 and (2.10) or that $s^* < q$ which is impossible (see e.g. [Zennaro 1986]).

With $C(1)$ or $C(2)$ we can use the second part of Theorem 2.12. Thus, there is a set, S_L, which contains exactly two indices. Furthermore, stages $i \notin S_L$ satisfy $C(q-1)$. We assume without loss of generality that $u_i \neq 0$ for $i \in S_L$. Notice that by combining the two order conditions of order $k+1$ in Theorem 2.12 one gets $\sum_{i \in S_L} b_i(\theta) u_i \equiv 0$. Using this for CMIRK schemes at $\theta = 1$, (2.12) reads

$$\sum_{i \in S_L} u_i (A - \lambda I) e_i = \sum_{i \in S_L} u_i (X - \lambda I) e_i = 0.$$

Let $j = \min\{i : i \in S_L\}$. Since X is strictly lower-triangular, and since $u_j \neq 0$ it follows that $\lambda = 0$ and $x_{j+1,j} = 0$. Moreover, for CMIRK schemes, the first stage satisfies $C(k)$ for arbitrary k, so we need not consider $1 \in S_L$. Also, since the first three stages of a CMIRK scheme cannot all satisfy $C(4)$ we only have to investigate the cases where stage 2, stage 3, or both are contained in S_L. Before we proceed with this, consider the $C(1)$ case. Since it is necessary that $\mathrm{rank}(G_5(A)) = 6$, we get, by using the condition corresponding to the tree $[[\tau],[\tau]]$, that

$$c^4 - 4(Ac)^2 = \xi(c^2 - 2Ac) = \xi \sum_{i \in S_L} u_i e_i,$$

for some $\xi \in R$. Hence

$$\xi \sum_{i \in S_L} u_i e_i = 2c^2(c^2 - 2Ac) - (c^2 - 2Ac)^2 = 2c_i^2 \sum_{i \in S_L} u_i e_i - \sum_{i \in S_L} u_i^2 e_i.$$

Since $u_i \neq 0$ for $i \in S_L$ we get $u_i = u_j$ for $i, j \in S_L$ when only $C(1)$ is satisfied.

(i) $\{2,3\} \subset S_L$. $x_{32} = 0$ with $c_2 = c_3$ and either of the conditions $C(2)$ or $u_2 = u_3$ implies that rows 2 and 3 are identical.

(ii) $2 \in S_L$, $3 \notin S_L$. Since $x_{32} = 0$ we can permute the second and third stage to obtain one of the cases below.

(iii) $\{3,4\} \subset S_L$. $x_{43} = 0$. In the $C(1)$ case the conditions $c_3 = c_4$, $u_3 = u_4$, immediately implies that stage 3 and 4 are identical. In the $C(1)$ case we compute u_j and $w_j = c_j^4 - \sum_{l=1}^{s} a_{jl} c_l^3$ to obtain

$$u_j = c_3^2(c_3 - 1) - x_{j2}, \quad w_j = c_3^2(c_3^2 - 1) - 2x_{j2}, \quad j = 3, 4.$$

By Theorem 2.12, (2.11) it is necessary that $w_j = \beta_4 u_j$ for some $\beta_4 \in R$. Imposing this with the above formulas we get

$$c_3^2(c_3 - 1)^2(x_{42} - x_{32}) = 0.$$

If $x_{42} = x_{32}$ then it is easy to see that stage 3 and 4 are identical. Since $C(4)$ holds for stage 1 and 2, we have $c_1 = 0$ and $c_2 = 1$ (or vice versa) such that $c_3 \in \{0, 1\}$ would imply $s^* < 5$, which is impossible.

(iv) $\{3, j\} \subset S_L, j > 4$. $x_{43} = 0$ so we may permute stage 3 and stage 4. The first 3 stages of an irreducible CMIRK scheme cannot satisfy $C(4)$, [Burrage, Chipman, Muir 1991]. ∎

In particular, this theorem shows that all 5th order CMIRK schemes with 6 stages satisfy $C(3)$. Turning to the order 6 case we have

Theorem 3.2 There are no 6th order CMIRK schemes with 7 stages or less.

Proof. By (2.10) a 6th order scheme must have at least 7 stages. Assume that such a scheme exists with 7 stages. Then, according to Theorem 3.1 it must satisfy $C(3)$ and we may apply the second part of Theorem

2.12 with $k = 4$. There is a set, S_L, that consists of exactly two indices. At least one of these must be in $\{1, 2, 3\}$ since stage i satisfies $C(5)$ for $i \notin S_L$. But neither stage 1 or stage 2 is of interest since both these stages satisfy $C(k)$ for arbitrary k when $C(3)$ is imposed. Thus, we must have $S_L = \{3, j\}$ where $j > 3$. Hence, $x_{43} = 0$. If $j = 4$ then $c_3 = c_4$ and stages 3 and 4 are identical. If $j > 4$ we permute the 3rd and 4th stage, and hence, the first 3 stages must satisfy $C(5)$ which is impossible. ∎

Hence, CMN(6) ≥ 8, and in Section 4 we shall see that CMIRK schemes of order 6 with 8 stages exist, thus CMN(6)=8.

Summarizing, we have the following table, where p is the order, CMN(p) is the minimal number of stages a CMIRK scheme of order p can have, and MN(p) is the minimal number of stages a (discrete) MIRK scheme of order p can have [Burrage, Chipman, Muir 1991].

p	CMN(p)	MN(p)
1	1	1
2	2	1
3	3	2
4	4	3
5	6	4
6	8	5

4. Characterizations of Continuous Mono-Implicit Runge-Kutta Schemes

In this section we present characterizations for a number of families of low order CMIRK schemes, having uniform orders p = 1, 2, 3, 4, 5, and 6, respectively. We consider only schemes having minimal number of stages and within each such class we will consider all possible $C(\xi)$ restrictions which preserve the minimal stage requirement. All the CMIRK schemes presented here having order 4,5 or 6, and all schemes of order 3 satisfying $C(3)$, are C^1 continuous. In fact, when the order is 3 or greater, it can be easily shown that for all CMIRK schemes which use only the minimal number of stages and satisfy $C(3)$, we must have C^1 continuity.

4.1. CMIRK schemes of order 1

A CMIRK scheme of uniform order 1 can be obtained using 1 stage. For the family of 1-stage CMIRK schemes we have the tableau,

$$\begin{array}{c|c|c} c & c & 0 \\ \hline & & b(\theta) \end{array}$$

where $b(\theta) = \theta$ and c is a free parameter. These schemes satisfy $C(1)$ and include the continuous versions of the explicit and implicit Euler schemes.

4.2. CMIRK schemes of order 2

A CMIRK of order 2 can be obtained using 2 stages. If we assume that only the $C(1)$ condition holds, we get the following 3-parameter family of 2-stage CMIRK schemes, of uniform order 2.

$$
\begin{array}{c|c|cc}
c_1 & c_1 & 0 & 0 \\
c_2 & v_2 & c_2 - v_2 & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta)
\end{array}
$$

where $c_1 \neq c_2$,

$$
b_1(\theta) = \frac{\theta}{c_2 - c_1}\left(c_2 - \frac{\theta}{2}\right) \quad \text{and} \quad b_2(\theta) = \frac{\theta}{c_1 - c_2}\left(c_1 - \frac{\theta}{2}\right).
$$

If we further require the schemes to satisfy $C(2)$, we get the following 1-parameter family of CMIRK schemes having uniform order 2,

$$
\begin{array}{c|c|cc}
0 & 0 & 0 & 0 \\
c_2 & {c_2}^2 & c_2(1 - c_2) & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta)
\end{array}
$$

where $c_2 \neq 0$,

$$
b_1(\theta) = \frac{\theta}{c_2}\left(c_2 - \frac{\theta}{2}\right) \quad \text{and} \quad b_2(\theta) = \frac{\theta^2}{2c_2}.
$$

This family includes the continuous version of the trapezoidal rule.

4.3. CMIRK schemes of order 3

A third order CMIRK scheme requires at least three stages. Furthermore, in order to have no more than 3 stages, it must satisfy $C(2)$. Therefore we will consider CMIRK schemes satisfying $C(2)$ and $C(3)$. For the $C(2)$ case we get the following 3 parameter family of schemes.

$$
\begin{array}{c|c|ccc}
0 & 0 & 0 & 0 & 0 \\
c_2 & {c_2}^2 & c_2(1 - c_2) & 0 & 0 \\
c_3 & v_3 & c_3 - v_3 - \dfrac{{c_3}^2 - v_3}{2c_2} & \dfrac{{c_3}^2 - v_3}{2c_2} & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta) & b_3(\theta)
\end{array}
$$

where

$$
b_1(\theta) = \frac{\theta(6c_2c_3 - 3\theta(c_2 + c_3) + 2\theta^2)}{6c_2c_3}, \quad b_2(\theta) = \frac{\theta^2(3c_3 - 2\theta)}{6c_2(c_3 - c_2)}, \quad \text{and} \quad b_3(\theta) = \frac{\theta^2(3c_2 - 2\theta)}{6c_3(c_2 - c_3)},
$$

and c_2, c_3, and v_3 are the parameters, with the restrictions that $c_2 \neq c_3 \neq 0$.

Let us now consider the case were we impose the maximum $C(3)$ condition. The CMIRK scheme tableau is further restricted and we get the following 1-parameter family,

$$
\begin{array}{c|c|ccc}
0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 \\
c_3 & {c_3}^2(3-2c_3) & c_3(c_3-1)^2 & c_3^2(c_3-1) & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta) & b_3(\theta)
\end{array}
$$

where $c_3 \neq 0, 1$ and

$$b_1(\theta) = \frac{\theta(6c_3 - 3\theta(1+c_3) + 2\theta^2)}{6c_3}, \quad b_2(\theta) = \frac{\theta^2(3c_3 - 2\theta)}{6(c_3-1)}, \quad \text{and} \quad b_3(\theta) = \frac{\theta^2(2\theta-3)}{6c_3(c_3-1)}.$$

This family includes the continuous version of the 3-point Lobatto rule.

4.4. CMIRK schemes of order 4

A CMIRK scheme of uniform order 4 can have the minimum number of stages, 4, if and only if it satisfies $C(3)$. Below we give a 3-parameter family of 4-stage, continuous 4-th order CMIRK schemes satisfying $C(3)$.

$$
\begin{array}{c|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 \\
c_3 & c_3^2(3-2c_3) & c_3(c_3-1)^2 & c_3^2(c_3-1) & 0 & 0 \\
c_4 & v_4 & \dfrac{\alpha}{6c_3} & \dfrac{\gamma}{6(c_3-1)} & \dfrac{-3(c_4^2-v_4)+2(c_4^3-v_4)}{6c_3(c_3-1)} & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta) & b_3(\theta) & b_4(\theta)
\end{array}
$$

where

$$b_1(\theta) = \frac{-\theta(3\theta^3 - 4\theta^2(1+c_3+c_4) + 6\theta(c_3+c_4+c_3c_4) - 12c_3c_4)}{12c_3c_4},$$

$$b_2(\theta) = \frac{\theta^2(3\theta^2 - 4\theta(c_3+c_4) + 6c_3c_4)}{12(c_3-1)(c_4-1)}, b_3(\theta) = \frac{\theta^2(3\theta^2 - 4\theta(c_4+1) + 6c_4)}{12c_3(c_3-1)(c_3-c_4)},$$

$$b_4(\theta) = \frac{\theta^2(3\theta^2 - 4\theta(c_3+1) + 6c_3)}{12c_4(c_4-1)(c_4-c_3)},$$

with $\alpha = 6c_3(c_4-v_4) - 3c_3(c_4^2-v_4) - 3(c_4^2-v_4) + 2(c_4^3-v_4)$, $\gamma = 3c_3(c_4^2-v_4) - 2(c_4^3-v_4)$, and the restrictions that $c_3 \neq c_4 \neq 0, 1$. In this case $F_4(A)$ is a vandermonde system over the abscissa $\{0, 1, c_3, c_4\}$ and the resultant weights, above, can be seen to satisfy

$$b_r(\theta) = \int_0^\theta L_r(t)dt, \quad r = 1, 2, 3, 4,$$

where $L_r(t)$ is the rth Lagrange interpolating polynomial for the abscissa set $\{c_1 = 0, c_2 = 1, c_3, c_4\}$, defined as follows. $L_r(t)$ is the unique 4th degree polynomial in t satisfying, for $r = 1, 2, 3, 4$,

$$L_r(c_r) = 1, \quad L_r(c_j) = 0, \qquad j = 1, \ldots, 4; j \neq r.$$

4.5. CMIRK schemes of order 5

As we saw in section 3, it is when we consider 5th order schemes that we first encounter the situation where it is no longer possible to find CMIRK schemes having the same number of stages as the uniform order. In fact, a CMIRK scheme of uniform order 5 must have at least 6 stages, and, by Theorem 3.1, must satisfy $C(3)$ in order to reach this minimum. If we simply apply the $C(3)$ conditions plus the order conditions up to and including order 5, we will get a 10 parameter family of CMIRK schemes, but the expressions for the coefficients and weights of the family are long, complicated expressions. However, for a given choice of the 10 free parameters it is trivial to obtain the corresponding CMIRK scheme.

We can simplify things slightly by imposing a restriction on this family of CMIRK schemes. We require all stages except the third to satisfy C(4). This reduces the number of degrees of freedom in the family and leaves us with a 7 parameter family of 6-stage, 5th order CMIRK schemes, which we present below.

$$\begin{array}{c|c|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
c_3 & c_3^2(3-2c_3) & c_3(c_3-1)^2 & c_3^2(c_3-1) & 0 & 0 & 0 & 0 \\
c_4 & \dfrac{c_4^2(3c_4^2 - 4c_3c_4 + 6c_3 - c_4)}{2c_3 - 1} & x_{41} & x_{42} & x_{43} & 0 & 0 & 0 \\
c_5 & v_5 & x_{51} & x_{52} & x_{53} & x_{54} & 0 & 0 \\
c_6 & v_6 & x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta) & b_3(\theta) & b_4(\theta) & b_5(\theta) & b_6(\theta)
\end{array}$$

where

$$x_{41} = \frac{c_4(c_4-1)^2(4c_3^2 - 3c_3c_4 - 2c_3 + c_4)}{2c_3(2c_3-1)}, \qquad x_{42} = \frac{c_4^2(c_4-1)(4c_3^2 - 3c_3c_4 + 2c_4 - 3c_3)}{2(c_3-1)(2c_3-1)},$$

$$x_{43} = \frac{c_4^2(c_4-1)^2}{2c_3(c_3-1)(2c_3-1)},$$

$$x_{51} = \frac{12c_3c_4(c_5 - v_5) - 6(c_3 + c_4 + c_3c_4)(c_5^2 - v_5) + 4(c_3 + c_4 + 1)(c_5^3 - v_5) - 3(c_5^4 - v_5)}{12c_3c_4},$$

$$x_{52} = -\frac{6c_3c_4(c_5^2 - v_5) - 4(c_3 + c_4)(c_5^3 - v_5) + 3(c_5^4 - v_5)}{12(c_3-1)(c_4-1)},$$

$$x_{53} = \frac{6c_4(c_5^2 - v_5) - 4(c_4+1)(c_5^3 - v_5) + 3(c_5^4 - v_5)}{12c_3(c_3-1)(c_3-c_4)},$$

$$x_{54} = \frac{6c_3(c_5^2 - v_5) - 4(c_3+1)(c_5^3 - v_5) + 3(c_5^4 - v_5)}{12c_4(c_4-1)(c_4-c_3)},$$

$$x_{62} = \frac{12c_3c_4c_5(c_6 - v_6 - x_{61}) - 6(c_3c_4 + c_3c_5 + c_4c_5)(c_6^2 - v_6) + 4(c_3+c_4+c_5)(c_6^3 - v_6) - 3(c_6^4 - v_6)}{12(c_3-1)(c_4-1)(c_5-1)},$$

$$x_{63} = \frac{12c_4c_5(c_6 - v_6 - x_{61}) - 6(c_4 + c_5 + c_4c_5)(c_6^2 - v_6) + 4(1+c_4+c_5)(c_6^3 - v_6) - 3(c_6^4 - v_6)}{12(1-c_3)(c_4-c_3)(c_5-c_3)},$$

$$x_{64} = \frac{12c_3c_5(c_6 - v_6 - x_{61}) - 6(c_3 + c_5 + c_3c_5)(c_6^2 - v_6) + 4(1+c_3+c_5)(c_6^3 - v_6) - 3(c_6^4 - v_6)}{12(1-c_4)(c_3-c_4)(c_5-c_4)},$$

and

$$x_{65} = \frac{12c_3c_4(c_6 - v_6 - x_{61}) - 6(c_3 + c_4 + c_3c_4)(c_6^2 - v_6) + 4(1+c_3+c_4)(c_6^3 - v_6) - 3(c_6^4 - v_6)}{12(1-c_5)(c_3-c_5)(c_4-c_5)},$$

The restrictions on the parameters c_3, c_4, c_5, and c_6 are that they must be distinct and not equal to 0 or 1.

The weights are determined by the rows of $F_5(A)$. We perform an elimination step on the row of $F_5(A)$ corresponding to the single non-quadrature condition, as follows. Replace

$$(Xc^3 + v/4) \quad \text{with} \quad c^4 - 4(Xc^3 + v/4).$$

This makes the right hand sides corresponding to this row equal to 0, and allows us to observe that the C(4) condition applied to all but the 3rd stage implies that the new row reduces to the form

$$[\begin{array}{cccccc} 0 & 0 & c_3^4 - 4([Xc^3]_3 + v_3/4) & 0 & 0 & 0 \end{array}],$$

where $[Xc^p]_j$ is the jth component of the vector Xc^p. Since the right hand sides for this row are all 0, this implies that all the coefficients for the third weight are zero, i.e. $b_3(\theta) = 0$, as given above. Furthermore, if we then remove the third column and this non-quadrature row from $F_5(A)$, the result is a vandermonde system over the abscissa $\{0, 1, c_4, c_5, c_6\}$. The resultant weight expressions are given by

$$b_r(\theta) = \int_0^\theta L_r(t)dt, \quad r = 1,2, \qquad b_3(\theta) = 0, \qquad b_r(\theta) = \int_0^\theta L_{r-1}(t)dt, \quad r = 4,5,6,$$

where $L_r(t)$ is the rth Lagrange interpolating polynomial over the abscissa set $\{0, 1, c_4, c_5, c_6\}$, defined as follows. Let $\psi_1 = 0$, $\psi_2 = 1$, $\psi_3 = c_4$, $\psi_4 = c_5$, and $\psi_5 = c_6$. Then $L_r(t)$ is the unique polynomial in t of degree 5 or less satisfying, for $r = 1, \ldots, 5$,

$$L_r(\psi_r) = 1, \qquad L_r(\psi_j) = 0, \quad j = 1, \ldots, 5; j \neq r.$$

4.6. CMIRK schemes of order 6

From Theorem 3.2 of the previous section, we saw that a CMIRK scheme of order 6 must have at least 8 stages. In this subsection we will construct a family of 8-stage CMIRK schemes of order 6, satisfying $C(3)$. The situation here is somewhat different than in the previous cases we have considered for lower orders because when we apply the $C(3)$ assumptions to the continuous order conditions up to and including order

6, we are left with 10 rather than 8 conditions. If we are to obtain a family of CMIRK schemes of order 6 with only 8 stages we must choose some of our free parameters to ensure that the 10 order conditions lead to only 8 independent rows in $G_6(A)$ and not less than 8 independent rows in $F_6(A)$. In the following discussion we outline one strategy for the determination of the coefficients of the CMIRK schemes which allows us to achieve this goal. Of the 10 order conditions present, 6 are quadrature conditions, and there are 4 non-quadrature conditions, having the following form,

$$b(\theta)^T(Xc^3+v/4)=\theta^5/20, \quad b(\theta)^Tc(Xc^3+v/4)=\theta^6/24,$$

$$b(\theta)^T(Xc^4+v/5)=\theta^6/30, \quad b(\theta)^T(X(Xc^3+v/4)+v/20)=\theta^6/120.$$

Our strategy involves forcing the 4 non-quadrature conditions to reduce to only 2 independent rows. In order to simplify the discussion, we first perform an elimination step on the 4 rows of $G_6(A)$ corresponding to the non-quadrature conditions. From each non-quadrature row we subtract a multiple of the corresponding quadrature row, and they scale the resulting row. The resulting rows in $F_6(A)$ are

$$\text{(i)} \quad c^5-4(Xc^3+v/4), \quad \text{(ii)} \quad c^6-4c(Xc^3+v/4),$$

$$\text{(iii)} \quad c^6-5(Xc^4+v/5), \quad \text{(iv)} \quad c^6-20(X(Xc^3+v/4)+v/20),$$

and the corresponding right-hand sides are 0. This simplification has also been used in [Verner 1990]. We now give a description of the strategy for the determination of the 8-stage, 6th order CMIRK family.

The first step follows from an idea of the previous subsection. Here we begin by imposing the restriction that all stages except the third and fourth satisfy the C(4) conditions. It can then be shown, from an inspection of the resultant forms of the order conditions, that it follows that the C(5) condition must also hold for all but the third and fourth stages. The rows of $F_6(A)$ derived from the above non-quadrature conditions become

$$\text{(i)} \quad [\begin{array}{cccccccc} 0 & 0 & u_3 & u_4 & 0 & 0 & 0 & 0 \end{array}], \qquad \text{(ii)} \quad [\begin{array}{cccccccc} 0 & 0 & c_3u_3 & c_4u_4 & 0 & 0 & 0 & 0 \end{array}],$$

$$\text{(iii)} \quad [\begin{array}{cccccccc} 0 & 0 & w_3 & w_4 & 0 & 0 & 0 & 0 \end{array}], \qquad \text{(iv)} \quad [\begin{array}{cccccccc} r_1 & r_2 & r_3 & r_4 & r_5 & r_6 & r_7 & r_8 \end{array}],$$

where $u_j=c_j^4-4([Xc^3]_j+v_j/4), j=3,4,\ w_j=c_j^5-5([Xc^4]_j+v_j/5), j=3,4,\ r_j=5(u_3x_{j3}+u_4x_{j4}), j=1,2,5,6,7,8$ and $r_j=w_j+5(u_3x_{j3}+u_4x_{j4}), j=3,4$. If we can force the last of the above rows to also have non-zeros in only positions 3 and 4, then we will have 4 rows with that same structure, of which exactly two must be independent. These two rows together with the 6 rows corresponding to the quadrature conditions will allow us to determine a family of 8 stage, 6th order schemes. Thus, our strategy reduces to determining coefficients of the family so that

$$r_1=r_2=r_5=r_6=r_7=r_8=0.$$

It follows immediately from the strictly lower triangular structure of X that $r_1=r_2=0$. It is also possible to satisfy the remaining conditions and we get some restrictions on some of the coefficients of the family. We are left with a 9-parameter family of 8-stage, 6th order CMIRK schemes. This defines the c, v, and X coefficients in terms of $c_3, c_4, c_5, c_6, c_7, v_7, c_8, v_8$ and x_{81}. We next consider the determination of the weights, $b_j(\theta), j=1,..,8$. These depend on the rows of $F_6(A)$.

Within $F_6(A)$, there are 6 rows corresponding to the quadrature conditions, plus the two independent rows, with non-zeros only in positions 3 and 4, corresponding to the reduced non-quadrature conditions. There is no need to work out the actual values for w_3, w_4 or r_3, r_4 since the values of the non-zeros in the two independent rows are not relevant. Since the right hand sides of these rows are zero for all orders, it can be observed that the two independent rows having non-zeros in only the third and fourth positions imply that all the coefficients corresponding to $b_3(\theta)$ and $b_4(\theta)$ must be zero, i.e. $b_3(\theta)=b_4(\theta)=0$. It then follows from Lemma 2.11 that,

$$b_r(\theta)=\int_0^\theta L_r(t)dt,\ r=1,2, \qquad b_3(\theta)=b_4(\theta)=0, \qquad b_r(\theta)=\int_0^\theta L_{r-2}(t)dt,\ r=5,6,7,8,$$

where $L_r(\theta)$ is the rth Lagrange interpolating polynomial for the abscissa $\{0, 1, c_5, c_6, c_7, c_8\}$, defined as follows. Let $\psi_1 = 0$, $\psi_2 = 1$, $\psi_3 = c_5$, $\psi_4 = c_6$, $\psi_5 = c_7$, and $\psi_6 = c_8$. Then $L_r(t)$ is the unique polynomial in t of degree 6 or less satisfying, for $r = 1, \ldots, 6$,

$$L_r(\psi_r) = 1, \qquad L_r(\psi_j) = 0, \quad j = 1, \ldots, 6;\ j \neq r.$$

In summary, a family of 6th order, 8-stage CMIRK schemes can be obtained by expressing some of the coefficients for each stage in terms of others of that stage using the C(3) conditions for stages 3 and 4, and the C(5) conditions for the remaining stages. Further relationships among the coefficients of the stages are obtained by requiring $r_5 = r_6 = r_7 = r_8 = 0$, as given earlier in this subsection. The completion of this process allows us to write all the c, v, and x coefficients in terms of the 9 free parameters, $c_3, c_4, c_5, c_6, c_7, v_7, c_8, v_8$ and x_{81}. The definition of the CMIRK family is completed by determining the weight polynomials in terms of the integrals of the Legendre polynomials, as indicated above. We have applied this approach and have set up and solved the above conditions to explicitly obtain expressions for all the coefficients and weight polynomials of this family. As might be expected, the coefficients of this CMIRK family are very long and complicated expressions so we do not present them here. Rather, we have arbitrarily selected values for the free parameters, inserted these values into the expressions for the coefficients and weight polynomials, and below display the resultant 8-stage, 6th order CMIRK scheme. The existence of this scheme establishes the order barrier for 6th order CMIRK schemes at 8.

$$\begin{array}{c|c|cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{8} & \frac{11}{256} & \frac{49}{512} & \frac{-7}{512} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{7}{8} & \frac{1813}{1280} & \frac{203}{512} & \frac{-609}{2560} & \frac{-7}{10} & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{4} & \frac{37}{928} & \frac{387}{12992} & \frac{39}{12992} & \frac{159}{182} & \frac{-15}{812} & 0 & 0 & 0 & 0 \\
\frac{3}{4} & \frac{441}{928} & \frac{1791}{12992} & \frac{-877}{12992} & \frac{-265}{812} & \frac{25}{812} & \frac{1}{2} & 0 & 0 & 0 \\
\frac{2}{5} & \frac{2}{5} & \frac{694}{109375} & \frac{-8114}{328125} & \frac{265424}{1640625} & \frac{-5008}{328125} & \frac{566}{46875} & \frac{-10954}{78125} & 0 & 0 \\
\frac{3}{5} & \frac{3}{5} & 0 & \frac{-37292}{815625} & \frac{204368}{1359375} & \frac{-3856}{271875} & \frac{-88514}{815625} & \frac{-550682}{3171875} & \frac{8756}{45675} & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta) & b_3(\theta) & b_4(\theta) & b_5(\theta) & b_6(\theta) & b_7(\theta) & b_8(\theta)
\end{array}$$

where

$$b_1(\theta) = \frac{-\theta}{216}(-216 + 1134\theta - 2968\theta^2 + 4113\theta^3 - 2880\theta^4 + 800\theta^5),$$

$$b_2(\theta) = \frac{\theta^2}{216}(108 - 684\theta + 1713\theta^2 - 1920\theta^3 + 800\theta^4),$$

$$b_3(\theta) = 0, \quad b_4(\theta) = 0,$$

$$b_5(\theta) = \frac{64\theta^2}{189}(54 - 234\theta + 411\theta^2 - 330\theta^3 + 100\theta^4), \quad b_6(\theta) = \frac{-64\theta^2}{189}(18 - 110\theta + 261\theta^2 - 270\theta^3 + 100\theta^4),$$

$$b_7(\theta) = \frac{-125\theta^2}{1512}(270 - 1440\theta + 2865\theta^2 - 2496\theta^3 + 800\theta^4),$$

$$b_8(\theta) = \frac{-125\theta^2}{1512}(180 - 1060\theta + 2385\theta^2 - 2304\theta^3 + 800\theta^4).$$

5. Conclusions

In this paper we have derived families of continuous mono-implicit Runge-Kutta schemes which use an optimal minimal number of stages, for orders 1 through 6. The underlying theoretical investigation has explored the relationship between the stage order and minimal number of stages required to obtain schemes of a desired order of accuracy, in the more general setting of continuous implicit Runge-Kutta schemes. Applications of these general results to the particular family of continuous mono-implicit Runge-Kutta schemes lead to the order barriers upon which the derivations of the families were based.

For orders 1 through 4 complete characterizations of the continuous mono-implicit families are presented. For order 5 a complete characterization is available but in the interest of shortening the presentation a somewhat restricted subfamily is presented. For the 6th order case, a particular strategy is used to obtain a family of schemes. The particular families presented in this paper for the 4th, 5th, and 6th order cases are interesting because they can be viewed as instances of continuous schemes derived from the more traditional interpolation-based approach for the construction of continuous extensions to Runge-Kutta schemes. In each of these cases, the stages which do not satisfy $C(p-1)$ for the pth order family, have zero weight polynomials. This leads to schemes which are similar to those discussed in [Enright et. al. 1986].

The schemes developed in this paper are complementary to those discussed in [Pruess 1986] since they require neither higher derivative evaluations nor function evaluations outside the current subinterval. The one-step aspect of these schemes is particularly important when we consider applying them in a parallel computing environment where one would like to be able to perform the work on each subinterval in parallel. An application of the characterizations of these continuous families is in the determination of particular continuous mono-implicit Runge-Kutta schemes for use in a defect-controlled boundary value ODE solver [Enright and Muir 1991]. After establishing suitable criteria for the selection of optimal schemes for this application, the next step will be to explore the parameter spaces of these families in order to compare various schemes and ultimately select good schemes of each order for implementation.

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