Optimal discrete and continuous mono-implicit Runge–Kutta schemes for BVODEs *

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Received December 1996; revised November 1998
Communicated by W.H. Enright

Recent investigations of discretization schemes for the efficient numerical solution of boundary value ordinary differential equations (BVODEs) have focused on a subclass of the well-known implicit Runge–Kutta (RK) schemes, called mono-implicit RK (MIRK) schemes, which have been employed in two software packages for the numerical solution of BVODEs, called TWPBVP and MIRKDC. The latter package also employs continuous MIRK (CMIRK) schemes to provide C^1 continuous approximate solutions. The particular schemes implemented in these codes come, in general, from multi-parameter families and, in some cases, do not represent optimal choices from these families. In this paper, several optimization criteria are identified and applied in the derivation of optimal MIRK and CMIRK schemes for orders 1–6. In some cases the schemes obtained result from the analysis of existent multi-parameter families; in other cases new families are derived from which specific optimal schemes are then obtained. New MIRK and CMIRK schemes are presented which are superior to those currently available. Numerical examples are provided to demonstrate the practical improvements that can be obtained by employing the optimal schemes.

Keywords: Runge–Kutta schemes, boundary value ODEs, efficiency

AMS subject classification: 65L05, 65L10

1. Introduction

Systems of boundary value ordinary differential equations (BVODEs) arise in a wide variety of applications – see [1, section 1.2]. In this paper we will assume two-point boundary value problems written in first order system form with boundary conditions,

$$y'(t) = f\big(t, y(t)\big), \qquad g\big(y(a), y(b)\big) = 0, \tag{1}$$

* This work was supported by the Natural Sciences and Engineering Research Council of Canada.

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where $t \in [a,b]$, $y:\mathbb{R} \to \mathbb{R}^n$, $f:\mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$, and $g:\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$. We refer the reader to [1, section 1.1] for a description of various classes of BVODEs and a discussion of how they can be converted to the form given in (1). Necessary and sufficient conditions for the existence and uniqueness of solutions to (1) are discussed in [1, section 3.1].

Numerical algorithms for the solution of BVODEs can generally be divided into two classes, initial value methods and global methods. The former class includes the well-known multiple shooting methods and is considered in [1, chapter 4]. The global methods include algorithms that employ finite difference, collocation, or Runge–Kutta schemes and are discussed in [1, chapter 5].

Runge–Kutta (RK) schemes (see, e.g., [5]), originally developed for the numerical solution of initial value ODE problems, have also been considered for use in the numerical solution of BVODEs for some time (see, e.g., [31], which also establishes the inclusion of the collocation schemes, for the problem class (1), within the class of RK schemes). More recent work has focused on a subclass of the implicit RK schemes called mono-implicit Runge–Kutta (MIRK) schemes (see [4,7–9,13,17,21]). Specific A-stable, symmetric schemes from this subclass have been employed in two recently developed software packages for the numerical solution of BVODEs, called TWPBVP [11] and MIRKDC [15]. The latter package also employs continuous MIRK (CMIRK) schemes to provide C^1 continuous approximate solutions. In many cases, the MIRK schemes employed in TWPBVP and MIRKDC are from the multi-parameter families given in [4] and the CMIRK schemes employed in MIRKDC are from the multi-parameter families given in [22]. MIRK schemes have also been considered for the numerical solution of stiff initial value ODEs [2,6,10]. (See [5] for discussion of symmetric, A-stable, and L-stable RK schemes.)

In this paper we identify several optimization criteria relevant in the context of deriving MIRK schemes for the numerical solution of BVODEs. These criteria include consideration of efficiency, stability, order, stage order, local error coefficients, and symmetry. Where possible, they will be applied to the families of [4,22] in order to allow the selection of specific schemes. However, in some instances, it will be necessary to derive families outside the scope considered in [4,22], before applying the optimization criteria.

This paper is organized as follows. In section 2, we review notation and results for MIRK and CMIRK schemes, and in section 3 we motivate the selection of the optimization criteria. In sections 4–9, we present analyses of families of discrete and continuous MIRK schemes of orders 1–6 in which we apply the optimization criteria to derive specific optimal MIRK and CMIRK schemes. In section 10, we provide numerical examples to examine the impact of the use of some of the new optimal schemes within the MIRKDC code. Section 11 gives our conclusions.

2. MIRK and CMIRK schemes

Here we give a brief summary of the notation and results from [4,22], to which we refer the reader for further details.

We assume that the problem interval $[a,b]$ is subdivided by a mesh $\{t_i\}_{i=0}^N$, with $a = t_0 < t_1 < \cdots < t_N = b$. In the BVODE context, a discrete numerical solution, $y_i \approx y(t_i)$, $i = 0, \ldots, N$, is obtained by applying Newton's method to the nonlinear system of equations consisting of the boundary condition equations and n more equations per subinterval which depend on the RK scheme. When the RK scheme is a MIRK scheme, the set of n equations associated with the ith subinterval has the form

$$y_i - y_{i-1} - h\sum_{r=1}^{s} b_r k_r = 0, \tag{2}$$

where

$$k_r = f\left(t_{i-1} + c_r h, (1-v_r)y_{i-1} + v_r y_i + h\sum_{j=1}^{r-1} x_{rj}k_j\right). \tag{3}$$

The scheme is defined by the number of stages, s, the coefficients, $\{v_r\}_{r=1}^s$ and $\{x_{rj}\}_{j=1,r=1}^{r-1,s}$, and the weights $\{b_r\}_{r=1}^s$. The abscissa, $\{c_r\}_{r=1}^s$, are defined by $c_r = v_r + \sum_{j=1}^{r-1} x_{rj}$. The length of the subinterval is $h = t_i - t_{i-1}$. The coefficients of a MIRK scheme are usually presented in a tableau of the form

$$\begin{array}{c|c|cccccc}
c_1 & v_1 & 0 & 0 & \ldots & \ldots & 0 \\
c_2 & v_2 & x_{21} & 0 & \ldots & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & & & \vdots \\
\vdots & \vdots & \vdots & & \ddots & & \vdots \\
c_s & v_s & x_{s1} & x_{s2} & \ldots & x_{s,s-1} & 0 \\
\hline
 & & b_1 & b_2 & \ldots & \ldots & b_s
\end{array}.$$

It is shown in [21] that the stability function for an MIRK scheme can be expressed in the form

$$R(z) = \frac{P(z, e-v)}{P(z,-v)} \quad \text{where } P(z,w) = 1 + zb^T(I - zX)^{-1}w,$$

$w \in \mathbb{R}^n$, $v = (v_1, \ldots, v_s)^T$, $b = (b_1, \ldots, b_s)^T$, X is an s by s matrix whose (r,j)th component is x_{rj}, and e is a vector of 1's of length s.

A MIRK scheme is of order p (i.e., has local error $p+1$) if for the local problem, $y'(t) = f(t, y(t))$, $y(t_{i-1}) = y_{i-1}$, the numerical solution, y_i, given by solving (2), satisfies $|y(t_i) - y_i| = \mathrm{O}(h^{p+1})$. A family of MIRK schemes of order p is derived by requiring its coefficients to satisfy a set of equations called order conditions. Since MIRK schemes can be expressed as IRK schemes [21], the order conditions for MIRK schemes are closely related to those for IRK schemes (see [4]). Specific order conditions will be presented as needed in later sections of this paper.

A pth order MIRK scheme has stage order q ($q \leqslant p$) if its coefficients satisfy the stage order conditions

$$Xc^{j-1} + \frac{v}{j} = \frac{c^j}{j}, \quad j = 1, \dots, q, \tag{4}$$

where $c^0 = e$ and $c^j = (c_1^j, \dots, c_s^j)^T$. When an RK scheme is applied to a system of stiff differential equations, an order reduction phenomenon (see, e.g., [18]) can cause a scheme having stage order q (with $q < p$) to behave as if its order were only q or $q+1$. Thus it can be important for a scheme to have as high a stage order as possible. However, in [4] it is proved that the maximum stage order of a pth order MIRK scheme is $\min(p, 3)$.

After the discrete solution is obtained, using a computation based on a MIRK scheme, a CMIRK scheme can be used on each subinterval to augment the discrete solution with a C^1 continuous interpolant over the whole problem interval. A CMIRK scheme applied on the subinterval $[t_{i-1}, t_i]$, is given, for $0 \leqslant \theta \leqslant 1$, by

$$u(t_{i-1} + \theta h) = y_{i-1} + h \sum_{r=1}^{s^*} b_r(\theta) k_r, \tag{5}$$

with the k_r's defined as in (3). In addition to the coefficients which define its stages, the scheme is defined by the weight polynomials, $\{b_r(\theta)\}_{r=1}^{s^*}$, which are polynomials in θ.

Some computational savings are achieved if the stages of the MIRK scheme can be stored and then reused by the CMIRK scheme. Thus there is an advantage to deriving CMIRK schemes with s stages identical to those of the MIRK scheme used before it. In this case the MIRK scheme is said to be "embedded" within the CMIRK scheme. Since some of the CMIRK families given in [22] make certain assumptions which do not hold for the MIRK schemes which we will embed, we will derive alternate versions of theses families in order to allow for the embedding of specific MIRK schemes.

A CMIRK scheme is of order p (i.e., has local error $p+1$) if for the local problem, $y'(t) = f(t, y(t))$, $y(t_{i-1}) = y_{i-1}$, with $u(t)$ as in (5), we have $\max_{0 \leqslant \theta \leqslant 1} |y(t_{i-1} + \theta h) - u(t_{i-1} + \theta h)| = \mathrm{O}(h^{p+1})$. A pth order CMIRK scheme is derived by requiring the coefficients and weight polynomials to satisfy continuous versions of the MIRK order conditions (see [22]). Specific continuous order conditions will be presented as needed in later sections of this paper. In addition, in order for the associated interpolant to have C^1 continuity, the weight polynomials must also satisfy certain continuity requirements (see [28]). Assuming that a discrete MIRK scheme with weights $\{b_r\}_{r=1}^{s}$ is embedded and that the first and second stages of the CMIRK scheme are $f(t_{i-1}, y_{i-1})$ and $f(t_i, y_i)$, respectively, the continuity conditions are

$$b_r(0) = 0, \quad b_r'(0) = \delta_{r1}, \quad b_r'(1) = \delta_{r2}, \quad b_r(1) = b_r, \quad r = 1, \dots, s^*, \tag{6}$$

where $b_r = 0$ if the rth stage is not an embedded stage, and δ_{rj} is the Kronecker delta. (For orders 1–3, an alternative approach to deriving a continuous scheme which leads to a C^1 interpolant is to construct the Hermite cubic interpolant, based on the four values, y_{i-1}, y_i, $f(t_{i-1}, y_{i-1})$ and $f(t_i, y_i)$. This gives

$$\widehat{u}(t_{i-1} + \theta h) = \widehat{b}_0(\theta) y_{i-1} + \widehat{b}_1(\theta) y_i + h\big(\widehat{d}_0(\theta) f(t_{i-1}, y_{i-1}) + \widehat{d}_1(\theta) f(t_i, y_i)\big), \qquad (7)$$

where $\widehat{b}_0(\theta) = (2\theta + 1)(\theta - 1)^2$, $\widehat{b}_1(\theta) = (3 - 2\theta)\theta^2$, $\widehat{d}_0(\theta) = \theta(\theta - 1)^2$, and $\widehat{d}_1(\theta) = \theta^2(\theta - 1)$. However, for each CMIRK scheme appearing in the sections on first, second, and third order schemes, it is always possible to rewrite this Hermite cubic interpolant so that it is equivalent to the CMIRK scheme. That is, each of these CMIRK schemes is actually the Hermite cubic interpolant (7) written in CMIRK form (5), using the embedded discrete MIRK scheme.)

The interpolant can be used to obtain an estimate of the defect $u'(t) - f(t, u(t))$, the amount by which the approximate solution fails to satisfy the ODE. It is sometimes possible to employ an interpolant whose local error is one order lower than that of the associated discrete scheme but in the context of defect control (as employed in MIRKDC) the order of the MIRK and CMIRK schemes must be the same [12]. Thus, in this paper, each MIRK scheme will be embedded in a CMIRK scheme of the same order.

3. Optimization criteria

The criteria to be used in the optimization of the general families of discrete MIRK schemes are:

(i) minimization of the number of stages,

(ii) requirement of symmetry/A-stability or one-sidedness/L-stability,

(iii) maximization of the overall stage order,

(iv) maximization of the stage order of individual stages, and

(v) minimization of the local error coefficient.

(i) The computational effort associated with the use of a MIRK scheme is dependent on the number of stages the scheme uses and thus it is important that s be as small as possible. In [4] it is proved that a pth order MIRK scheme always requires at least $p - 1$ stages, and for MIRK schemes of orders 1 through 6, it is always possible to achieve this lower bound (when maximization of order for a given number of stages is the only criterion). However, some of the other optimization criteria may force a scheme to use one or more extra stages.

(ii) There is considerable literature on the use of symmetric, A-stable schemes in the solution of BVODEs (see, e.g., [1, chapter 10]). The usual definition of symmetry for an RK scheme (see [26]) requires the scheme to be equal to its reflection [25]. The reflection of an RK scheme is the scheme obtained by applying the original scheme in the reverse direction on the same subinterval. This means swapping t_{i-1} and t_i, y_{i-1} and y_i, and replacing h by $-h$ in (2), (3). As discussed in [26], in order for a RK scheme to be symmetric it must be possible to map each stage, under the reflection transformation, into another stage (or observe that it is invariant under the reflection transformation, in which case the stage maps into itself). The MIRK scheme tableau is a particularly convenient representation for the investigation of symmetry; a symmetric MIRK scheme can be characterized by a specially structured tableau in which pairs of stages map into each other or individual stages map into themselves, under the reflection transformation. In the derivation of symmetric MIRK schemes we will begin with a general form for the tableau which ensures symmetry and then apply the order conditions and other criteria to determine specific values for the free coefficients. Since symmetric schemes must have even order (see [26]), these derivations will be considered in the sections on second, fourth, and sixth order schemes. All derived schemes will be A-stable.

There has also been some investigation of the use of one-sided, L-stable schemes in the numerical solution of BVODEs (see, e.g., [1, chapter 10; 3,19]). One-sided schemes have the property that the degree of the numerator and denominator of the stability function of the scheme are different (usually by one). Such a scheme can be used to introduce growth (upwinding) or damping in the numerical solution. We will impose the one-sided condition by requiring the stability function of the family we derive to have a denominator whose degree is one greater than that of the numerator (a damped scheme). This gives a family of one-sided (damped) schemes; the reflection of this family gives a complementary family of one-sided (upwinded) schemes. (In [26] it is shown that if $R(z)$ is the stability function of an RK scheme, then $R(-z)^{-1}$ is the stability function of its reflection.) All derived schemes will be L-stable.

(iii), (iv) Although the maximum overall stage order of a pth order MIRK scheme is min$(p, 3)$, when there are sufficient free parameters, it may be possible to impose higher stage order on some of the stages of the MIRK scheme. The presence of these high order stages can lead, for the CMIRK scheme within which the MIRK scheme is to be embedded, to a simpler derivation and simpler expressions for the weight polynomials (see, e.g., [20]). The usual notation for recording the stage order conditions satisfied by each of the s stages of a MIRK scheme uses a stage order vector [29], SOV $= (q_1, q_2, \ldots, q_s)$, where q_r is the stage order of the rth stage.

(v) For a pth order MIRK family, the accuracy of the scheme depends on the principal error coefficient of h^{p+1} in the local truncation error [5]. The dependence of this coefficient on the parameters of the RK scheme can be expressed in terms of the (appropriately weighted) unsatisfied order conditions for order $p+1$ (see, e.g., [5] and references within). The square root of the sum of the squares of these quantities is defined to be C_{p+1}. Letting C_{p+2} be the corresponding quantity for the O(h^{p+2}) term, we will require C_{p+1} to be minimized subject to the condition that C_{p+2}/C_{p+1} is not too large. A scheme with a smaller C_{p+1} value will tend to have a smaller local error and thus may be more accurate than another scheme of the same order with a larger C_{p+1} value. The improved accuracy can lead to a more efficient solution since it may be possible to employ larger subintervals. It is important that the ratio C_{p+2}/C_{p+1} be not too large because otherwise the error from the O(h^{p+2}) term can dominate the error from the O(h^{p+1}) term, negating the potential improvement associated with the small C_{p+1} value. These computations are done using MAPLE [30] and the FORTRAN RKTREE package [23].

To some extent these criteria are in competition; for example, the requirement that a scheme be one-sided might force it to employ more stages than the minimum required to achieve a given order. In the investigation of some of the classes of schemes presented in this paper, we will consider schemes which use one or two extra stages to meet various criteria. This idea is discussed in [24] for explicit RK schemes.

We will embed each MIRK scheme in a CMIRK scheme of the same order, which we will then optimize according to most of the same criteria discussed above. Criterion (i) is addressed in [22]; a pth order CMIRK scheme requires at least p stages but this lower bound cannot be met for $p \geqslant 5$. Criteria (ii) and (iii) are not relevant for CMIRK schemes. Criterion (iv) can help to reduce the complexity of the derivation of the CMIRK scheme and the complexity of the expressions for the resultant weight polynomials. For criterion (v), similar comments hold for the continuous MIRK schemes: a more accurate interpolant may be obtained when the free coefficients are chosen to minimize C_{p+1}, assuming the C_{p+2} coefficient does not become too large. Furthermore, when defect control is employed, the additional coefficients, C'_{p+1} and C'_{p+2}, associated with the O(h^p) and O(h^{p+1}) terms in the local expansion of the defect (see [12]) are relevant. The accuracy of the defect estimate may be improved when the coefficients of the interpolant are also chosen to minimize C'_{p+1}, provided C'_{p+2}/C'_{p+1} does not become too large.

4. First order, one-sided schemes

When the first order, 1-stage, family of MIRK schemes of [4] is required to be one-sided, the one free parameter, c_1, must equal 0 or 1, giving the explicit and implicit Euler schemes, respectively. The latter scheme is L-stable, has stage order 1, the SOV = (1), $C_2 = 0.50$, and $C_3 \approx 0.90$, with $C_3/C_2 \approx 1.8$. A first order CMIRK scheme which leads to a C^1 interpolant and which contains embedded within it the backward Euler scheme has the tableau

$$\begin{array}{c|c|cc} 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \hline & & b_1(\theta) & b_2(\theta) \end{array}, \tag{8}$$

where $b_1(\theta) = \theta(\theta - 1)^2$ and $b_2(\theta) = -\theta^2(\theta - 2)$. These weight polynomials are determined by applying the continuity requirements (6). The scheme also satisfies the continuous order condition for first order, $b(\theta)^T e = \theta$, and has the SOV = $(1, 1)$. This scheme has $C_2 = 0.50$, $C_3 \approx 0.90$, $C_3/C_2 \approx 1.8$, $C'_2 \approx 0.75$, $C'_3 \approx 1.3$, and

$C_3'/C_2' \approx 1.7$. It is obtained with no extra stage evaluations, since the endpoint stages from the discrete scheme can be shared by adjacent subintervals.

5. Second order schemes

5.1. One-sided schemes

Since the only 1-stage, second order, MIRK scheme is symmetric, we begin here with the general 2-stage MIRK family. Application of the order conditions for second order, $b^T e = 1$ and $b^T c = \frac{1}{2}$, and the stage order 2 conditions, (4) with $q = 2$, gives a family with free parameter $c_2 \neq 1$. It is one-sided provided $c_2 = 0$ and the SOV $= (2, 2)$. Since it is possible to choose c_2 to make this a third order scheme, C_3 can be made arbitrarily small (and thus C_4/C_3 arbitrarily large). However, in order to obtain a second order, one-sided scheme, we will choose c_2 so that $C_4/C_3 \approx 2.0$; we choose $c_2 = \frac{2}{7}$ and then $C_3 \approx 0.017$ and $C_4 \approx 0.035$. The tableau and stability function are

$$\begin{array}{c|c|cc} 1 & 1 & 0 & 0 \\ \frac{2}{7} & \frac{24}{49} & -\frac{10}{49} & 0 \\ \hline & & \frac{3}{10} & \frac{7}{10} \end{array} \quad \text{and} \quad R(z) = \frac{\frac{5}{14}z + 1}{\frac{1}{7}z^2 - \frac{9}{14}z + 1}. \tag{9}$$

This scheme is L-stable. A C^1 interpolant is obtained by embedding (9) in a second order CMIRK scheme having the tableau

$$\begin{array}{c|c|ccc} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ \frac{2}{7} & \frac{24}{49} & 0 & -\frac{10}{49} & 0 \\ \hline & & \theta(\theta-1)^2 & \frac{1}{10}\theta^2(4\theta-1) & -\frac{7}{10}\theta^2(2\theta-3) \end{array}.$$

The weight polynomials are chosen to satisfy the continuity conditions (6). The scheme also satisfies the continuous order conditions for first and second order, $b(\theta)^T e = \theta$ and $b(\theta)^T c = \frac{1}{2}\theta^2$, and has the SOV $= (2, 2, 2)$, $C_3 \approx 0.017$, $C_4 \approx 0.035$, $C_4/C_3 \approx 2.0$, $C_3' \approx 0.025$, $C_4' \approx 0.069$, and $C_4'/C_3' \approx 2.8$. This scheme is obtained with no extra stage evaluations since the endpoint stages can be shared among adjacent subintervals.

5.2. Symmetric schemes

The general form for the tableau of a symmetric, 1-stage MIRK scheme is

$$\begin{array}{c|c|c} \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & & b_1 \end{array}.$$

It has stage order 1 and the SOV $= (1)$. Application of the order condition for first order, $b^T e = 1$, gives $b_1 = 1$, the midpoint scheme [2], which is also the 1-point Gauss collocation scheme [5]. This scheme is A-stable and has $C_3 \approx 0.093$, $C_4 \approx 0.088$, and

$C_4/C_3 \approx 0.95$. A C^1 interpolant can be obtained by embedding the midpoint scheme in a second order CMIRK scheme having the tableau

$$\begin{array}{c|c|ccc} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \hline & & \theta(\theta-1)^2 & \theta^2(\theta-1) & -\theta^2(2\theta-3) \end{array}.$$

The weight polynomials are chosen to satisfy the continuity conditions (6). The scheme also satisfies the continuous order conditions for first and second order. It has the SOV $= (2,2,1)$, $C_3 \approx 0.093$, $C_4 \approx 0.088$, $C_4/C_3 \approx 0.95$, $C_3' \approx 0.14$, $C_4' \approx 0.15$, and $C_4'/C_3' \approx 1.0$. Since endpoint stages from adjacent subintervals can be shared, the cost is only one extra stage evaluation per subinterval.

We briefly consider using an extra stage to obtain a MIRK scheme having the maximum stage order 2. The general form for the tableau of a symmetric, 2-stage MIRK scheme is

$$\begin{array}{c|c|cc} c_1 & c_1 & 0 & 0 \\ 1-c_1 & 1-c_1 & 0 & 0 \\ \hline & & b_1 & b_1 \end{array},$$

with $c_1 \neq \frac{1}{2}$. Imposing stage order 2, (4) with $q = 2$, and the order condition for first order, $b^T e = 1$, gives $c_1 = 0$ and $b_1 = \frac{1}{2}$, which gives the second order trapezoidal scheme [2], also known as the 2-point Lobatto collocation scheme [5] for which $C_3 \approx 0.12$, $C_4 \approx 0.18$, and $C_4/C_3 \approx 1.5$ and the SOV $= (2,2)$. A C^1 interpolant is obtained when the trapezoidal scheme is embedded within a CMIRK scheme with the tableau (8) with $b_1(\theta) = -\frac{1}{2}\theta(\theta-2)$ and $b_2(\theta) = \frac{1}{2}\theta^2$. These weight polynomials are chosen to satisfy the continuity conditions (6). The scheme also satisfies the continuous order conditions for first and second order. The SOV $= (2,2)$ and $C_3 \approx 0.12$, $C_4 \approx 0.18$, $C_4/C_3 \approx 1.5$, $C_3' \approx 0.18$, $C_4' \approx 0.27$, and $C_4'/C_3' \approx 1.5$. This scheme is obtained without the need for any extra stages. In fact, since adjacent subintervals can share endpoint stages, the trapezoidal scheme can be implemented for the same cost as the midpoint scheme.

Table 1
Summary of second order schemes.

Type	MIRK schemes			CMIRK schemes		
	s	q	C_3	s^*	C_3	C_3'
O	2	2	0.017	3	0.017	0.025
S	1	1	0.093	3	0.093	0.14
S	2	2	0.12	2	0.12	0.18

5.3. Summary of second order schemes

In table 1 we summarize the MIRK and CMIRK schemes of second order, derived in this section. The *Type* is O for one-sided or S for symmetric, s is the number of stages of the MIRK scheme, q is its stage order, and s^* is the number of stages of the CMIRK scheme within which the MIRK scheme is embedded.

6. Third order, one-sided schemes

We begin with the one-parameter, 2-stage, third order, MIRK family presented in [4], and require the scheme be one-sided; this forces the single free parameter c_1 to equal 0 or 1 and increases the stage order to 2. For these choices of c_1, the family reduces to two specific MIRK schemes identified in [2]. They are reflections of each other and are equivalent to the 2-point Radau collocation schemes [5]. For $c_1 = 1$, the scheme is L-stable. It has the SOV $= (3, 2)$ and $C_4 \approx 0.024$, $C_5 \approx 0.035$, $C_5/C_4 \approx 1.4$. An interpolant with C^1 continuity is obtained by embedding this scheme in a third order CMIRK scheme which is an instance of the third order CMIRK family given in [22]; the tableau is

$$\begin{array}{c|c|ccc}
0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 \\
\frac{1}{3} & \frac{5}{9} & 0 & -\frac{2}{9} & 0 \\
\hline
 & & \theta(\theta-1)^2 & \frac{1}{4}\theta^2(2\theta-1) & -\frac{3}{4}\theta^2(2\theta-3)
\end{array} .$$

The weight polynomials, chosen to satisfy the continuous order conditions up to order three, which for a stage order 2 scheme are $b(\theta)^T e = \theta$, $b(\theta)^T c = \frac{1}{2}\theta^2$, and $b(\theta)^T c^2 = \frac{1}{3}\theta^3$, also satisfy the continuity conditions (6). This CMIRK scheme has the SOV $=(3, 3, 2)$. Since the embedded MIRK scheme includes one of the endpoints of the subinterval, the CMIRK scheme is obtained with no extra stage evaluations required. For this CMIRK scheme, $C_4 \approx 0.024$, $C_5 \approx 0.035$, $C_5/C_4 \approx 1.4$, $C_4' \approx 0.043$, $C_5' \approx 0.063$, and $C_5'/C_4' \approx 1.5$.

We next consider using an extra stage to increase the stage order. We first impose the requirements that the scheme employ three stages, be of third order, have stage order 2, and be one-sided. The resultant scheme is given in [4], with the restriction that $\{1, c_2, c_3\}$ be distinct, and is one-sided provided $c_2 \neq 0, \frac{1}{3}$, and $v_3 \neq c_3(2 - c_3)$. When we attempt to increase the stage order of this scheme, we find that this requires $c_2 = 0$, which violates the condition for the scheme to be one-sided.

Thus in order to derive a third order, stage order 3, one-sided scheme, we must use four stages. We begin with a general 4-stage MIRK family, and apply the stage order 3 conditions, (4) with $q = 3$, and the order conditions for third order, which for stage order 3 schemes are $b^T e = 1$, $b^T c = \frac{1}{2}$, and $b^T c^2 = \frac{1}{3}$. The resultant scheme has free parameters c_3, c_4, v_4 and b_4. We then choose v_4 and b_4 to obtain a one-sided family, with $c_3 \neq 0, 1$, $c_4 \neq 0, 1$, and $c_3 \neq c_4$. An analysis of C_4 and C_5 for this family shows that $C_4 \approx 0.048$, for all c_3, c_4, and that although C_5 is minimized for $c_3 = c_4 = 0$, its value does not vary much for $0 \leqslant c_3,\ c_4 \leqslant 1$; acceptable ratios of C_5/C_4 are obtained for all such c_3 and c_4 values. We derived the CMIRK family containing this family of MIRK scheme and found similar results. Therefore we can simply choose c_3 and c_4 to avoid the singularities arising in the expressions for the b_r's; these are the restricted values mentioned above. We will do this by choosing c_3 and c_4 to minimize $\|b\|_2$. This gives $c_3 = \frac{3}{4}$ and $c_4 = \frac{1}{5}$ and we get a MIRK scheme with tableau and stability function

$$\begin{array}{c|c|cccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ \frac{3}{4} & \frac{27}{32} & \frac{3}{64} & -\frac{9}{64} & 0 & 0 \\ \frac{1}{5} & \frac{13}{125} & \frac{16}{125} & -\frac{4}{125} & 0 & 0 \\ \hline & & \frac{5}{9} & -\frac{3}{8} & \frac{128}{99} & -\frac{125}{264} \end{array} \quad \text{and} \quad R(z) = \frac{\frac{1}{3}z + 1}{\frac{1}{6}z^2 - \frac{2}{3}z + 1}. \tag{10}$$

It is L-stable, has stage order 3, the SOV $= (3,3,3,3)$, $C_4 \approx 0.048$, $C_5 \approx 0.086$, and $C_5/C_4 \approx 2.0$. A C^1 interpolant can be obtained from a third order CMIRK scheme which contains the stages of (10). The tableau is

$$\begin{array}{c|c|cccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ \frac{3}{4} & \frac{27}{32} & \frac{3}{64} & -\frac{9}{64} & 0 & 0 \\ \frac{1}{5} & \frac{13}{125} & \frac{16}{125} & -\frac{4}{125} & 0 & 0 \\ \hline & & -\frac{1}{9}\theta(\theta^2+3\theta-9) & \frac{1}{8}\theta^2(14\theta-17) & -\frac{128}{99}\theta^2(2\theta-3) & \frac{125}{264}\theta^2(2\theta-3) \end{array}.$$

The weight polynomials are chosen to satisfy the continuity conditions (6). The scheme also satisfies the continuous order conditions up to third order. It has $C_4 \approx 0.048$, $C_5 \approx 0.086$, $C_4' \approx 0.085$, and $C_5' \approx 0.14$. This gives $C_5/C_4 \approx 2.0$ and $C_5'/C_4' \approx 1.6$. It has the SOV $= (3,3,3,3)$.

6.1. *Summary of third order schemes*

In table 2 we summarize the MIRK and CMIRK schemes of third order, derived in this section.

Table 2
Summary of third order schemes.

Type	MIRK schemes			CMIRK schemes		
	s	q	C_4	s^*	C_4	C_4'
O	2	2	0.024	3	0.024	0.043
O	4	3	0.048	4	0.048	0.085

7. Fourth order schemes

7.1. One-sided schemes

We begin with a family of three stage, fourth order, stage order two, MIRK schemes given in [4]. This family is one-sided provided its one free parameter $c_2 \neq 0$. If we attempt to apply the stage order three conditions to this family we find that we must have $c_2 = 0$, and the scheme is no longer one-sided. We next consider four stage methods in order to attempt to derive one-sided, fourth order, stage order three, schemes. A general family of four stage, fourth order, stage order three, schemes is given in [4]. However, an examination of its stability function shows that it is impossible to choose the free parameters so that a one-sided scheme is obtained.

We thus turn to using five stages to derive a one-sided, fourth order scheme with stage order 3. Beginning with the general 5-stage MIRK family, we apply the stage order 3 conditions, (4) with $q = 3$, and the order conditions up to order 4, which for stage order 3 schemes, are $b^T e = 1$, $b^T c = \frac{1}{2}$, $b^T c^2 = \frac{1}{3}$, and $b^T c^3 = \frac{1}{4}$. We also maximize the stage order of the fifth stage by applying the stage order 4 condition to it. (The first two stages have stage order 4; the third and fourth stages have their maximum stage order 3.) We then impose the one-sided requirement. The resultant family has SOV $= (4, 4, 3, 3, 4)$ and free parameters c_3, c_4, c_5, b_5, with the requirement that $\{0, 1, c_3, c_4\}$ be distinct. It is one-sided provided $b_5 \neq 0$. C_5 for this scheme can be made arbitrarily small since it is possible to choose the free parameters to achieve fifth order. We will attempt to choose the free parameters to make C_5 small while keeping C_6/C_5 from getting too large. A numerical search of the parameter space shows that the choices $c_3 = 1/20$, $c_4 = 19/20$, $c_5 = \frac{1}{2}$, and $b_5 = \frac{1}{2}$, minimize $C_5 \approx 0.00030$, give $C_6 \approx 0.00052$, and $C_6/C_5 \approx 1.7$. The tableau and stability function of the resultant scheme are

$$\begin{array}{c|c|ccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{20} & \frac{29}{4000} & \frac{361}{8000} & -\frac{19}{8000} & 0 & 0 & 0 \\
\frac{19}{20} & \frac{3971}{4000} & \frac{19}{8000} & -\frac{361}{8000} & 0 & 0 & 0 \\
\frac{1}{2} & \frac{11}{16} & \frac{1}{32} & \frac{267}{608} & \frac{25}{684} & -\frac{25}{36} & 0 \\
\hline
 & & -\frac{43}{228} & -\frac{43}{228} & \frac{25}{57} & \frac{25}{57} & \frac{1}{2}
\end{array} \tag{11}$$

and

$$R(z) = \frac{1 + \frac{13}{32}z + \frac{5}{9}z^2}{1 - \frac{19}{32}z + \frac{7}{84}z^2 - \frac{1}{64}z^3}.$$

This scheme is L-stable.

The five stages of (11) can be embedded in a five stage, fourth order, stage order three, CMIRK scheme; thus for this CMIRK scheme we have an SOV $= (4, 4, 3, 3, 4)$. The weight polynomials of the scheme are chosen to satisfy the C^1 continuity conditions (6) as well as the continuous order conditions up to order, which for a stage order 3 scheme, are $b(\theta)^T e = \theta$, $b(\theta)^T c = \frac{1}{2}\theta^2$, $b(\theta)^T c^2 = \frac{1}{3}\theta^3$, and $b(\theta)^T c^3 = \frac{1}{4}\theta^4$. This leaves one free parameter, the coefficient of the θ^4 term in $b_5(\theta)$. An analysis of C_5 shows that choosing this coefficient to be zero gives optimal results. The tableau of this CMIRK scheme is

$$\begin{array}{c|c|ccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{20} & \frac{29}{4000} & \frac{361}{8000} & -\frac{19}{8000} & 0 & 0 & 0 \\
\frac{19}{20} & \frac{3971}{4000} & \frac{19}{8000} & -\frac{361}{8000} & 0 & 0 & 0 \\
\frac{1}{2} & \frac{11}{16} & \frac{1}{32} & \frac{267}{608} & \frac{25}{684} & -\frac{25}{36} & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta) & b_3(\theta) & b_4(\theta) & b_5(\theta)
\end{array},$$

where

$$\begin{aligned}
b_1(\theta) &= -\frac{1}{228}\theta\left(1200\theta^3 - 2714\theta^2 + 1785\theta - 228\right), \\
b_3(\theta) &= \frac{25}{171}\theta^2\left(40\theta^2 - 86\theta + 49\right), \\
b_4(\theta) &= -\frac{25}{171}\theta^2\left(40\theta^2 - 74\theta + 31\right), \\
b_2(\theta) &= \frac{1}{228}\theta^2\left(1200\theta^2 - 2086\theta + 843\right),
\end{aligned}$$

and

$$b_5(\theta) = -\frac{1}{2}\theta^2(2\theta - 3).$$

It has $C_5 \approx 0.00085$, $C_6 \approx 0.0016$, $C_6/C_5 \approx 1.9$, $C_5' \approx 0.0052$, $C_6' \approx 0.0087$, $C_6'/C_5' \approx 1.7$.

7.2. *Symmetric schemes*

The general form for the tableau of a symmetric, 3-stage MIRK scheme is

$$\begin{array}{c|c|ccc}
c_1 & c_1 & 0 & 0 & 0 \\
1 - c_1 & 1 - c_1 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & x_{31} & -x_{31} & 0 \\
\hline
 & & b_1 & b_1 & b_3
\end{array}.$$

Imposing stage order 2, (4) with $q = 2$, and the order conditions for first order and third order, $b^T e = 1$ and $b^T c^2 = \frac{1}{3}$, gives $b_1 = \frac{1}{6}$, $b_3 = \frac{2}{3}$, $c_1 = 0$ and $x_{31} = \frac{1}{8}$, which gives the 3-stage, fourth order, MIRK scheme reported in [2]. This scheme also satisfies the stage order 3 conditions so it actually has stage order 3 and the SOV = $(4, 4, 3)$. It is A-stable and has $C_5 \approx 0.0057$, $C_6 \approx 0.0081$, and $C_6/C_5 \approx 1.4$. It is equivalent to the 3-point Lobatto collocation scheme [5]. (This is the fourth order MIRK scheme currently implemented in MIRKDC and TWPBVP.)

This scheme can be embedded in a fourth order, stage order 3, CMIRK family (a special case of the family from [22]). The free parameters are c_4 and v_4 with the restriction that $c_4 \neq 0, \frac{1}{2}, 1$. Further analysis shows that $C_5 \approx 0.0057$ for all $c_4 \in (0,1)$, $C_5' \approx 0.0090$ for $c_4 \in (\frac{1}{3}, \frac{2}{3})$, $C_6 \approx 0.0081$ for all $c_4 \in (0,1)$, C_6' is minimized for $c_4 \in (0.48, 0.52)$, and that none of these quantities depend on v_4. We must also avoid the singularities in the weight polynomials; we will do this by choosing c_4 to minimize $\|b(\theta)\|_2$. This occurs for $c_4 \in (0.1, 0.4)$. We can thus attain the minima for C_5, C_5', C_6, and $\|b(\theta)\|$ and nearly attain the minimum for C_6', by choosing $c_4 = \frac{2}{5}$. We then have $C_5 \approx 0.0057$ and $C_6 \approx 0.0081$ which give $C_6/C_5 \approx 1.4$ and $C_5' \approx 0.0090$, $C_6' \approx 0.015$, which gives $C_6'/C_5' \approx 1.7$. This analysis leaves v_4 free; we choose $v_4 = c_4$. The corresponding tableau is

$$
\begin{array}{c|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{8} & -\frac{1}{8} & 0 & 0 \\
\frac{2}{5} & \frac{2}{5} & \frac{17}{125} & -\frac{13}{125} & -\frac{4}{125} & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta) & b_3(\theta) & b_4(\theta)
\end{array}, \tag{12}
$$

where

$$
b_1(\theta) = -\frac{1}{12}\theta(3\theta-4)\big(5\theta^2-6\theta+3\big), \qquad b_2(\theta) = \frac{1}{6}\theta^2\big(5\theta^2-6\theta+2\big),
$$
$$
b_3(\theta) = -\frac{2}{3}\theta(3\theta-2)(5\theta-6), \qquad b_4(\theta) = \frac{125}{12}\theta^2(\theta-1)^2.
$$

This scheme provides a slight improvement over the one reported in [15] and currently implemented in MIRKDC. In that paper, the free parameters for the fourth order CMIRK scheme were given the values, $c_4 = \frac{3}{4}$ and $v_4 = \frac{27}{32}$, and then, $C_5 \approx 0.0057$, $C_6 \approx 0.0081$, $C_6/C_5 \approx 1.4$, $C_5' \approx 0.010$, $C_6' \approx 0.017$, $C_6'/C_5' \approx 1.7$. Comparing these values with those reported above for the optimal scheme (12), we see that C_5 and C_6 are the same while the C_5' and C_6' values are approximately 10% larger than those of the optimal scheme (12).

In appendix A.1, we derive a 4-stage, fourth order, stage order 3, MIRK scheme (and associated CMIRK scheme) whose C_5 value is smaller than that of the 3-point Lobatto collocation scheme. (Its data is included in the third line of table 3.)

7.3. *Summary of fourth order schemes*

In table 3 we summarize the MIRK and CMIRK schemes derived in this section. For comparison purposes, we also include data for the 2-point Gauss collocation scheme in the last line of the table. We note that since both stages are implicit, the cost per subinterval associated with this scheme is generally higher than for a MIRK scheme. Since the natural interpolant for the Gauss scheme is only second order and has only C^0 continuity, we do not include data for it. However, it is possible to use

Table 3
Summary of fourth order schemes.

Type	MIRK schemes			CMIRK schemes		
	s	q	C_5	s^*	C_5	C_5'
O	5	3	0.00030	5	0.00085	0.0052
S	3	3	0.0057	4	0.0057	0.0090
S	4	3	0.0048	4	0.0048	0.010
S	2	2	0.0043	–	–	–

the techniques considered in this paper to construct a fourth order CMIRK scheme for this Gauss scheme that gives a C^1 interpolant – see [16].

8. Fifth order, one-sided schemes

We begin with the family of 4-stage, fifth order, stage order 2, MIRK schemes given in [4] which has free parameters c_2 and c_3. It is one-sided provided $c_2 \neq 0$. If we attempt to increase the stage order to 3, we find that c_2 must be 0, and thus the scheme can no longer be one-sided.

We therefore consider 5-stage, fifth order, stage order 3, one-sided MIRK schemes, and return to the 5-stage, fourth order, stage order 3, one-sided MIRK family discussed in the previous section. Recall that this scheme has free parameters c_3, c_4, c_5, and b_5; it is possible to choose c_3 and b_5 to satisfy the fifth order conditions, which for stage order 3 schemes are $b^T c^4 = \frac{1}{5}$ and $b^T(Xc^3 + v/4) = \frac{1}{20}$. It is also possible to choose c_5 to make the fifth stage have stage order 5; thus the SOV $= (5, 5, 3, 3, 5)$. This scheme has c_4 free with the restrictions that $c_4 \neq 0, 1, \frac{1}{2}, \frac{3}{5}, \frac{21}{25}, \approx 0.44, \approx 0.84$, to avoid singularities in the expressions for the other coefficients.

Further analysis shows that reasonable values for C_6, C_7, and C_7/C_6 are obtained for all choices of c_4 that avoid the above restricted values and the region $(0.6, 0.84)$. We can choose c_4 to avoid the singularities in the b_r's by choosing c_4 to minimize $\|b\|_2$. This gives $c_4 = \frac{17}{20}$, which gives $C_6 \approx 0.0012$, $C_7 \approx 0.0029$ and $C_7/C_6 \approx 2.4$. The tableau of the resultant MIRK scheme is

$$\begin{array}{c|c|ccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 \\
-\frac{5}{28} + \frac{\sqrt{393}}{84} & v_3 & x_{31} & x_{32} & 0 & 0 & 0 \\
\frac{17}{20} & v_4 & x_{41} & x_{42} & 0 & 0 & 0 \\
\frac{125}{224} + \frac{\sqrt{393}}{224} & v_5 & x_{51} & x_{52} & x_{53} & x_{54} & 0 \\
\hline
 & & b_1 & b_2 & b_3 & b_4 & b_5
\end{array}, \tag{13}$$

where

$$v_3 = \frac{229}{686} - \frac{101\sqrt{393}}{6174}, \qquad x_{31} = -\frac{6409}{16464} + \frac{1097\sqrt{393}}{49392},$$

$$x_{32} = -\frac{2027}{16464} + \frac{299\sqrt{393}}{49392},$$
$$v_4 = \frac{3757}{4000}, \qquad x_{41} = \frac{153}{8000}, \qquad x_{42} = -\frac{867}{8000},$$
$$v_5 = \frac{237704435}{314703872} + \frac{1823343\sqrt{393}}{314703872}, \qquad x_{51} = \frac{223029279}{10699931648} - \frac{36659445\sqrt{393}}{10699931648},$$
$$x_{52} = -\frac{1758793}{629407744} - \frac{682877\sqrt{393}}{629407744}, \qquad x_{53} = \frac{164181897}{3862233088} + \frac{9504189\sqrt{393}}{3862233088},$$
$$x_{54} = -\frac{725872015625}{2815085142016} + \frac{2028935875\sqrt{393}}{2815085142016},$$
$$b_1 = -\frac{19}{272} - \frac{11\sqrt{393}}{816}, \qquad b_2 = \frac{3035}{28224} + \frac{187\sqrt{393}}{84672},$$
$$b_3 = \frac{43425027}{132009920} + \frac{2257089\sqrt{393}}{132009920},$$
$$b_4 = \frac{998000}{21897819} - \frac{550000\sqrt{393}}{65693457}, \qquad b_5 = \frac{5993083}{10195920} + \frac{25961\sqrt{393}}{10195920}.$$

The stability function is

$$R(z) = -\frac{\frac{1}{20}z^2 + \frac{2}{5}z + 1}{\frac{1}{60}z^3 - \frac{3}{20}z^2 + \frac{3}{5}z - 1}.$$

This scheme is L-stable.

It is shown in [22] that a fifth order, stage order 3 CMIRK scheme must employ at least 6 stages and such a family is given there. For that family, there is the additional assumption that stages 4–6 have stage order 4, and therefore that the CMIRK scheme have the SOV $= (5, 5, 3, 4, 4, 4)$. However, for (13), it was not possible to make the fourth stage have stage order 4. Thus we will embed the 5 stages from (13) in a 6 stage, fifth order, CMIRK scheme having a SOV $= (5, 5, 3, 3, 5, 5)$. The derivation is based on satisfying the continuous order conditions for fifth order, stage order 3 schemes, $b(\theta)^T e = \theta$, $b(\theta)^T c = \frac{1}{2}\theta^2$, $b(\theta)^T c^2 = \frac{1}{3}\theta^3$, $b(\theta)^T c^3 = \frac{1}{4}\theta^4$, $b(\theta)^T c^4 = \frac{1}{5}\theta^5$, and $b(\theta)^T(Xc^3 + \frac{v}{4}) = \frac{1}{20}\theta^5$, and is similar to that employed in [22]. Applying an elimination step to the last order condition above gives $b(\theta)^T(Xc^3 + v/4 - c^4/4) = 0$. Since $(Xc^3 + v/4 - c^4/4)$ is the vector of stage order conditions for stage order 4 (see (4)), only the third and fourth components are nonzero. The order condition reduces to

$$\frac{-119921 + 5947\sqrt{393}}{2765952} b_3(\theta) - \frac{2601}{640000} b_4(\theta) = 0,$$

giving $b_3(\theta)$ in terms of $b_4(\theta)$. The remaining five order conditions can then be used to determine the remaining weight polynomials. The resultant weight polynomials also satisfy the continuity conditions (6). The resultant CMIRK family has c_6 and v_6 as free parameters with the restrictions that $c_6 \neq 0, 1, (23-\sqrt{393})/20, (125+\sqrt{393})/224$.

Further analysis shows that for $c_6 \in (0.23, 0.86)$, we can achieve the minimum values $C_6 \approx 0.0012$ and $C_7 \approx 0.0029$; then $C_7/C_6 \approx 2.4$. The analysis for C_6' indicates that the choice of $c_6 = \frac{14}{25}$ provides the minimum value of $C_6' \approx 0.0022$; then $C_7' \approx 0.0055$, and $C_7'/C_6' \approx 2.5$, independently of the choice of v_6. With no restriction according to the criteria identified here, we choose $v_6 = c_6$.

The tableau of the resultant CMIRK scheme is

$$\begin{array}{c|c|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
c_3 & v_3 & x_{31} & x_{32} & 0 & 0 & 0 & 0 \\
c_4 & v_4 & x_{41} & x_{42} & 0 & 0 & 0 & 0 \\
c_5 & v_5 & x_{51} & x_{52} & x_{53} & x_{54} & 0 & 0 \\
\frac{14}{25} & \frac{14}{25} & x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta) & b_3(\theta) & b_4(\theta) & b_5(\theta) & b_6(\theta)
\end{array},$$

where the coefficients for the first five rows of the tableau are given in (13), and

$$x_{61} = -\frac{28017913\sqrt{393}}{4515625000} - \frac{493827103}{22578125000}, \qquad x_{62} = \frac{37817373}{2187500000} - \frac{745481\sqrt{393}}{19687500000},$$

$$x_{63} = \frac{13007794215933}{92082812500000} + \frac{686727625023\sqrt{393}}{92082812500000},$$

$$x_{64} = -\frac{2408972902336}{9694346953125} - \frac{2652451648\sqrt{393}}{5816608171875},$$

$$x_{65} = \frac{4506347288003}{40301953125000} - \frac{10198807509\sqrt{393}}{13433984375000},$$

$$\begin{aligned}
b_1(\theta) = {} & \frac{(42919\sqrt{393} + 726581)}{279890843022336}\theta\big(18537388880\theta^4 - 38982646641\theta^3 \\
& - 67451925\sqrt{393}\,\theta^3 + 17021879994\theta^2 + 176781154\sqrt{393}\,\theta^2 \\
& + 11276789925\theta - 160912047\sqrt{393}\,\theta - 1037557668 + 61288332\sqrt{393}\big),
\end{aligned}$$

$$\begin{aligned}
b_2(\theta) = {} & -\frac{-19675275 + 559079\sqrt{393}}{52326786664728576}\theta^2\big(42507897760\theta^3 - 54481638857\theta^2 \\
& + 177236475\sqrt{393}\,\theta^2 + 10096725582\theta - 284790018\sqrt{393}\,\theta \\
& + 702696666 + 128060898\sqrt{393}\big),
\end{aligned}$$

$$\begin{aligned}
b_3(\theta) = {} & -\frac{11675241621 + 610860615\sqrt{393}}{23449186109440}\theta^2\big(13440\theta^3 - 35583\theta^2 \\
& - 75\sqrt{393}\,\theta^2 + 156\sqrt{393}\,\theta + 320044\theta - 10500 - 84\sqrt{393}\big),
\end{aligned}$$

$$b_4(\theta) = \frac{5288000\sqrt{393} - 38154000}{364664379807}\theta^2\big(13440\theta^3 - 355583\theta^2 - 75\sqrt{393}\,\theta^2 + 156\sqrt{393}\,\theta + 320044\theta - 10500 - 84\sqrt{393}\big),$$

$$b_5(\theta) = -\frac{948114929207 + 39148987645\sqrt{393}}{169641265393978560}\theta^2\big(2297220\theta^3 + 294525\sqrt{393}\,\theta^2 - 10931079\theta^2 - 612612\sqrt{393}\,\theta + 155631192\theta - 7225680 + 329868\sqrt{393}\big),$$

$$b_6(\theta) = \frac{1944296875 + 59765625\sqrt{393}}{119925757952}(\theta - 1)^2\theta^2\big(896\theta - 1241 + 51\sqrt{393}\big).$$

8.1. Summary of fifth order schemes

In table 4 we summarize the MIRK and CMIRK schemes derived in this section. For comparison purposes, we also include data for the 3-stage Radau collocation scheme in the last line of the table. We note that since two of the stages are implicit, the cost per subinterval associated with this scheme is generally higher than for a MIRK scheme. Since the natural interpolant for the Radau scheme is only third order and has only C^0 continuity, we do not include data for it. However, it is possible to use the techniques considered in this paper to construct a fifth order CMIRK scheme for this Radau scheme that gives a C^1 interpolant – see also [16].

Table 4
Summary of fifth order schemes.

Type	MIRK schemes			CMIRK schemes		
	s	q	C_6	s^*	C_6	C_6'
O	5	3	0.0012	6	0.0012	0.0022
O	3	3	0.0010	–	–	–

9. Sixth order schemes

9.1. One-sided schemes

We first consider the family of five stage, sixth order, stage order three MIRK schemes given in [4]. However, an examination of the stability function shows that there are no one-sided schemes in this family. In appendix A.2 we consider this family further, with respect to criterion (iv).

We therefore consider 6-stage MIRK schemes. Beginning with the general family of such schemes, we impose stage order 3, (4) with $q = 3$, and the order conditions up to sixth order, which for a stage order 3 scheme are $b^Te = 1$, $b^Tc = \frac{1}{2}$, $b^Tc^2 = \frac{1}{3}$, $b^Tc^3 = \frac{1}{4}$, $b^Tc^4 = \frac{1}{5}$, $b^T(Xc^3 + v/4) = \frac{1}{20}$, $b^Tc^5 = \frac{1}{6}$, $b^T(Xc^4 + v/5) = \frac{1}{30}$, $b^Tc(Xc^3 + v/4) = \frac{1}{24}$, and $b^T(X(Xc^3 + v/4) + v/20) = \frac{1}{120}$. In order to reduce the complexity of the calculation, we choose c_3, c_4, and v_4 so that the third and fourth stages are equal to those of the 5-stage, sixth order, MIRK scheme of [2]. The remaining free parameters are chosen to make the fifth and sixth stages have stage order 4, and to ensure that the scheme is one-sided and L-stable. The resultant scheme has the SOV $= (6, 6, 3, 3, 4, 4)$ and the tableau and stability function

$$\begin{array}{c|c|cccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{4} & \frac{5}{32} & \frac{9}{64} & -\frac{3}{64} & 0 & 0 & 0 & 0 \\ \frac{3}{4} & \frac{27}{32} & \frac{3}{64} & -\frac{9}{64} & 0 & 0 & 0 & 0 \\ \frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{31-7\sqrt{5}}{50} & \frac{1}{25}+\frac{\sqrt{5}}{50} & \frac{4}{75}+\frac{\sqrt{5}}{50} & \frac{4}{75} & -\frac{4}{25} & 0 & 0 \\ \frac{1}{2}+\frac{\sqrt{5}}{10} & 1 & \frac{1}{180}-\frac{53\sqrt{5}}{4500} & -\frac{43}{450}-\frac{11\sqrt{5}}{2250} & x_{63} & x_{64} & x_{65} & 0 \\ \hline & & \frac{1}{12} & \frac{1}{12} & 0 & 0 & \frac{5}{12} & \frac{5}{12} \end{array}, \qquad (14)$$

where

$$x_{63} = \frac{8}{225} + \frac{124\sqrt{5}}{1125}, \qquad x_{64} = \frac{16}{225} - \frac{124\sqrt{5}}{1125}, \qquad x_{65} = -\frac{31}{60} + \frac{7\sqrt{5}}{60},$$

and

$$R(z) = \frac{\frac{-11+7\sqrt{5}}{2400}z^3 + \frac{-1+7\sqrt{5}}{300}z^2 + \frac{29+7\sqrt{5}}{120}z + 1}{\frac{31-7\sqrt{5}}{7200}z^4 + \frac{-113+21\sqrt{5}}{2400}z^3 + \frac{51-7\sqrt{5}}{200}z^2 + \frac{-91+7\sqrt{5}}{120}z + 1}.$$

This scheme has $C_7 \approx 0.00038$, $C_8 \approx 0.00060$, and $C_8/C_7 \approx 1.6$.

We will next embed (14) in a 9-stage, sixth order, stage order 3, CMIRK scheme. The three extra stages can be chosen to satisfy the stage order 6 conditions and thus the SOV $= (6, 6, 3, 3, 4, 4, 6, 6, 6)$. The derivation is given in appendix A.3. There are 7 free parameters, v_7, x_{71}, c_8, v_8, c_9, v_9, and x_{91}; a numerical search of the parameter space shows that an optimal choice for these coefficients is $v_7 = \frac{43}{50}$, $x_{71} = \frac{13}{500}$, $c_8 = \frac{6}{25}$, $v_8 = \frac{13}{200}$, $c_9 = \frac{43}{50}$, $v_9 = \frac{63}{100}$, and $x_{91} = \frac{29}{1000}$, and we get a scheme with the tableau

$$\begin{array}{c|c|ccccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{4} & \frac{5}{32} & \frac{9}{64} & \frac{-3}{64} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{4} & \frac{27}{32} & \frac{3}{64} & \frac{-9}{64} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c_5 & v_5 & x_{51} & x_{52} & x_{53} & x_{54} & 0 & 0 & 0 & 0 & 0 \\ c_6 & v_6 & x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{43}{50} & x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & 0 & 0 & 0 \\ \frac{6}{25} & \frac{13}{200} & x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & 0 & 0 \\ \frac{43}{50} & \frac{63}{100} & x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & 0 \\ \hline & & b_1(\theta) & b_2(\theta) & b_3(\theta) & b_4(\theta) & b_5(\theta) & b_6(\theta) & b_7(\theta) & b_8(\theta) & b_9(\theta) \end{array},$$

where the coefficients for the fifth and sixth rows are given in (14),

$$x_{71} = \frac{13}{500}, \qquad x_{72} = -\frac{43}{500}, \qquad x_{73} = -\frac{73}{250}, \qquad x_{74} = \frac{73}{250},$$

$$x_{75} = \frac{43\sqrt{5}}{200} - \frac{3}{20}, \qquad x_{76} = -\frac{3}{20} - \frac{43\sqrt{5}}{200},$$

$$x_{81} = \frac{323563423}{4687500000}, \qquad x_{82} = \frac{21465247}{4687500000}, \qquad x_{83} = \frac{27170304}{48828125},$$

$$x_{84} = -\frac{27170304}{48828125}, \qquad x_{85} = \frac{22480883}{187500000} - \frac{2141091\sqrt{5}}{9765625},$$

$$x_{86} = \frac{2141091\sqrt{5}}{9765625} + \frac{22480883}{187500000}, \qquad x_{87} = -\frac{1351584}{9765625},$$

$$x_{91} = \frac{29}{1000}, \qquad x_{92} = -\frac{31275464779}{961875000000}, \qquad x_{93} = \frac{518230396}{791015625},$$

$$x_{94} = -\frac{518230396}{791015625}, \qquad x_{95} = \frac{12115609721}{37125000000} - \frac{1201248227\sqrt{5}}{6187500000},$$

$$x_{96} = \frac{12115609721}{37125000000} + \frac{1201248227\sqrt{5}}{6187500000}, \qquad x_{97} = -\frac{131756267}{6855468750},$$

$$x_{98} = -\frac{140834677}{352123200},$$

$$b_1(\theta) = -\frac{\theta(20000\theta^5 - 137400\theta^4 + 314442\theta^3 - 328934\theta^2 + 1673670\theta - 38700)}{38700},$$

$$b_2(\theta) = \frac{\theta^2(585000\theta^4 - 1675200\theta^3 + 1767741\theta^2 - 816632\theta + 142416)}{39900},$$

$$b_3(\theta) = b_4(\theta) = 0, \qquad b_5(\theta) = \frac{\theta^2(5000\theta^4 - 15600\theta^3 + 17673\theta^2 - 8596\theta + 1548)}{60},$$

$$b_6(\theta) = \frac{\theta^2(5000\theta^4 - 15600\theta^3 + 17673\theta^2 - 8596\theta + 1548)}{60},$$

$$b_7(\theta) = -\frac{8\theta^2(\theta-1)^2(68125\theta^2 - 856750\theta + 25929)}{8775},$$

$$b_8(\theta) = -\frac{3125\theta^2(\theta-1)^2(5000\theta^2 - 5000\theta + 903)}{275652},$$

$$b_9(\theta) = -\frac{25000\theta^2(\theta-1)^2(625\theta^2 - 625\theta + 171)}{251937}.$$

It has $C_7 \approx 0.00038$, $C_8 \approx 0.00060$, $C_8/C_7 \approx 1.6$, $C_7' \approx 0.0021$, $C_8' \approx 0.0037$, $C_8'/C_7' \approx 1.8$.

9.2. Symmetric schemes

Imposition of the symmetry structure on the tableau of a general 5-stage MIRK scheme gives a tableau of the form

$$\begin{array}{c|c|ccccc} c_1 & v_1 & 0 & 0 & 0 & 0 & 0 \\ 1-c_1 & 1-v_1 & 0 & 0 & 0 & 0 & 0 \\ c_3 & v_3 & x_{31} & x_{32} & 0 & 0 & 0 \\ 1-c_3 & 1-v_3 & -x_{32} & -x_{31} & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & x_{51} & -x_{51} & x_{53} & -x_{53} & 0 \\ \hline & & b_1 & b_1 & b_3 & b_3 & b_5 \end{array}.$$

The application of the stage order 3 conditions, (4) with $q = 3$, and the first, third, and fifth order conditions, which for a stage order 3 scheme are $b^T e = 1$, $b^T c^2 = \frac{1}{3}$, $b^T c^4 = \frac{1}{5}$, $b^T(Xc^3 + \frac{v}{4}) = \frac{1}{20}$, leads to a one-parameter family with free parameter $c_3 \neq 0, 1, \frac{1}{2}$ or $\frac{1}{2} \pm \sqrt{5}/10$. It has stage order 3 and the stage order vector is $(6, 6, 3, 3, 3)$. C_7 is minimized when $c_3 = \frac{1}{2} \pm \sqrt{21}/14$, in which case $C_7 \approx 0.00025$, $C_8 \approx 0.00046$ and then $C_8/C_7 \approx 1.8$.

With $c_3 = \frac{1}{2} - \sqrt{21}/14$, we get a scheme whose tableau is

$$\begin{array}{c|c|ccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} - \frac{\sqrt{21}}{14} & \frac{1}{2} - \frac{9\sqrt{21}}{98} & \frac{1}{14} + \frac{\sqrt{21}}{98} & -\frac{1}{14} + \frac{\sqrt{21}}{98} & 0 & 0 & 0 \\ \frac{1}{2} + \frac{\sqrt{21}}{14} & \frac{1}{2} + \frac{9\sqrt{21}}{98} & \frac{1}{14} - \frac{\sqrt{21}}{98} & -\frac{1}{14} - \frac{\sqrt{21}}{98} & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & -\frac{5}{128} & \frac{5}{128} & \frac{7\sqrt{21}}{128} & -\frac{7\sqrt{21}}{128} & 0 \\ \hline & & \frac{1}{20} & \frac{1}{20} & \frac{49}{180} & \frac{49}{180} & \frac{16}{45} \end{array} \qquad (15)$$

and whose stability function is

$$R(z) = \frac{\frac{1}{120}z^3 + \frac{1}{10}z^2 + \frac{1}{2}z + 1}{-\frac{1}{120}z^3 + \frac{1}{10}z^2 - \frac{1}{2}z + 1}.$$

This scheme is A-stable.

The symmetric, 5-stage, sixth order MIRK scheme obtained by choosing $c_3 = \frac{1}{4}$ has appeared frequently in the literature, see, e.g., [2,4,9]. (It is the sixth order MIRK scheme currently implemented in TWPBVP and MIRKDC.) It has $C_7 \approx 0.00027$, $C_8 \approx 0.00048$. These are approximately 8 and 4%, respectively, larger than those of the optimal scheme (15).

It is shown in [22] that the minimum number of stages required for a sixth order CMIRK scheme is 8, and that such a scheme must have stage order 3. An example of an 8 stage, sixth order, stage order 3, family of CMIRK schemes is given in [22] but there the SOV is assumed to be $(5, 5, 3, 3, 5, 5, 5, 5)$. This rules out the possibility of embedding (15) or the symmetric, 5-stage, sixth order MIRK scheme with $c_3 = \frac{1}{4}$, mentioned above, within this CMIRK family, since in either case the fifth stage can have at most stage order 3. The symmetric, 5-stage, sixth order MIRK scheme (with $c_3 = \frac{1}{4}$) implemented in the MIRKDC code is embedded there in a 9-stage, sixth order, CMIRK scheme.

However, it is possible to derive an 8-stage, sixth order, stage order 3, CMIRK scheme, within which (15) is embedded. The derivation strategy is similar to one presented in [22] but with the slightly more general assumption that the fifth stage satisfies only the stage order 3 conditions. The derivation is given in appendix A.4. The resultant CMIRK scheme has the SOV $= (6, 6, 3, 3, 3, 5, 6, 6)$. There are four free parameters, v_6, v_7, c_8, and v_8, with the restrictions that $c_8 \neq 0, 1, \frac{1}{2}$, or $\frac{1}{2} \pm \sqrt{7}/14$.

An analysis of C_7 shows that choosing the lone free parameter upon which it depends, c_8, from the intervals $(0, 0.35)$ or $(0.9, 1)$ is optimal. Analysis of C'_7 shows that it is minimized for $c_8 \approx \frac{87}{100}$; this gives $C_7 \approx 0.00025$ and $C'_7 \approx 0.00053$. With this choice for c_8, we get $C_8 \approx 0.00047$, $C'_8 \approx 0.0012$, which gives $C_8/C_7 \approx 1.9$ and $C'_8/C'_7 \approx 2.2$. (C_8 and C'_8 do not depend on the remaining free parameters, v_6, v_7, and v_8.)

For the 9-stage CMIRK scheme reported in [15], the free coefficients were chosen somewhat arbitrarily. It has $C_7 \approx 0.0019$, $C_8 \approx 0.0032$, giving $C_8/C_7 \approx 1.7$, and $C'_7 \approx 0.0089$, $C'_8 \approx 0.015$, which gives $C'_8/C'_7 \approx 1.7$. We note that the corresponding values for the optimal scheme (16) are approximately 13, 15, 6, and 8%, respectively, of those of this 9-stage scheme. Furthermore, the optimal scheme uses one stage less.

Since none of C_7, C_8, C'_7, C'_8 depend on them, v_6, v_7, and v_8 are left free and we choose them equal to their corresponding abscissa values. The resultant CMIRK scheme has the tableau

$$
\begin{array}{c|c|cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} - \frac{\sqrt{21}}{14} & \frac{1}{2} - \frac{9\sqrt{21}}{98} & x_{31} & x_{32} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} + \frac{\sqrt{21}}{14} & \frac{1}{2} + \frac{9\sqrt{21}}{98} & x_{41} & x_{42} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & x_{51} & x_{52} & x_{53} & x_{54} & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & x_{61} & x_{62} & x_{63} & x_{64} & 0 & 0 & 0 & 0 \\
\frac{1}{2} - \frac{\sqrt{7}}{14} & \frac{1}{2} - \frac{\sqrt{7}}{14} & x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & 0 & 0 \\
\frac{87}{100} & \frac{87}{100} & x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & 0 \\
\hline
 & & b_1(\theta) & b_2(\theta) & b_3(\theta) & b_4(\theta) & b_5(\theta) & b_6(\theta) & b_7(\theta) & b_8(\theta)
\end{array}, \quad (16)
$$

where

$$
x_{31} = \frac{1}{14} + \frac{\sqrt{21}}{98}, \qquad x_{32} = -\frac{1}{14} + \frac{\sqrt{21}}{98},
$$

$$
x_{41} = \frac{1}{14} - \frac{\sqrt{21}}{98}, \qquad x_{42} = -\frac{1}{14} - \frac{\sqrt{21}}{98},
$$

$$
x_{51} = -\frac{5}{128}, \qquad x_{52} = \frac{5}{128}, \qquad x_{53} = \frac{7\sqrt{21}}{128}, \qquad x_{54} = -\frac{7\sqrt{21}}{128},
$$

$$x_{61} = \frac{1}{64}, \qquad x_{62} = -\frac{1}{64}, \qquad x_{63} = \frac{7\sqrt{21}}{192}, \qquad x_{64} = -\frac{7\sqrt{21}}{192},$$
$$x_{71} = \frac{3}{112} + \frac{9\sqrt{7}}{1960}, \qquad x_{72} = -\frac{3}{112} + \frac{9\sqrt{7}}{1960}, \qquad x_{73} = \frac{3\sqrt{7}\sqrt{3}}{112} + \frac{11\sqrt{7}}{840},$$
$$x_{74} = -\frac{3\sqrt{7}\sqrt{3}}{112} + \frac{11\sqrt{7}}{840}, \qquad x_{75} = \frac{88\sqrt{7}}{5145}, \qquad x_{76} = -\frac{18\sqrt{7}}{343},$$
$$x_{81} = \frac{2707592511}{1000000000000} - \frac{1006699707\sqrt{7}}{1000000000000},$$
$$x_{82} = -\frac{51527976591}{1000000000000} - \frac{1006699707\sqrt{7}}{1000000000000},$$
$$x_{83} = -\frac{610366393}{75000000000} + \frac{7046897949\sqrt{7}}{1000000000000} + \frac{14508670449\sqrt{7}\sqrt{3}}{1000000000000},$$
$$x_{84} = -\frac{610366393}{75000000000} + \frac{7046897949\sqrt{7}}{1000000000000} - \frac{14508670449\sqrt{7}\sqrt{3}}{1000000000000},$$
$$x_{85} = -\frac{12456457}{1171875000} + \frac{1006699707\sqrt{7}}{109375000000},$$
$$x_{86} = \frac{3020099121\sqrt{7}}{437500000000} + \frac{47328957}{625000000}, \qquad x_{87} = -\frac{7046897949\sqrt{7}}{250000000000},$$

and where

$$\begin{aligned}
b_1(\theta) = {} & -\frac{1}{2112984835740}\theta\bigl(1450\sqrt{7} + 12233\bigr)\bigl(800086000\theta^5 - 29366505584\theta^4 \\
& + 63579600\sqrt{7}\,\theta^4 - 201404565\sqrt{7}\,\theta^3 + 42351522620\theta^3 + 232506630\sqrt{7}\,\theta^2 \\
& - 30331093390\theta^2 + 11165116695\theta - 116253315\sqrt{7}\,\theta - 191568780 \\
& + 22707000\sqrt{7}\bigr),
\end{aligned}$$

$$\begin{aligned}
b_2(\theta) = {} & -\frac{-10799 + 650\sqrt{7}}{29551834260}\theta^2\bigl(249620000\theta^4 + 473200\sqrt{7}\,\theta^3 - 670243328\theta^3 \\
& + 666296000\theta^2 - 751855\sqrt{7}\,\theta^2 + 236210\sqrt{7}\,\theta - 295072500\theta + 5080365 \\
& + 50895\sqrt{7}\bigr),
\end{aligned}$$

$$b_3(\theta) = b_4(\theta) = \frac{49}{64}b_5(\theta),$$

$$\begin{aligned}
b_5(\theta) = {} & \frac{4144 + 800\sqrt{7}}{2231145}\theta^2\bigl(14000\theta^4 - 48216\theta^3 + 1200\sqrt{7}\,\theta^3 + 62790\theta^2 - 3555\sqrt{7}\,\theta^2 \\
& + 3610\sqrt{7}\,\theta - 37450\theta + 9135 - 1305\sqrt{7}\bigr),
\end{aligned}$$

$$\begin{aligned}
b_6(\theta) = {} & -\frac{-24332 + 2960\sqrt{7}}{1227278493}(\theta - 1)^2\theta^2\bigl(-1561000\theta^2 + 2461284\theta + 109520\sqrt{7}\,\theta \\
& - 86913\sqrt{7} - 979272\bigr),
\end{aligned}$$

$$b_7(\theta) = -\frac{49\sqrt{7}}{63747}(\theta - 1)^2\theta^2\left(20000\theta^2 - 20000\theta + 3393\right),$$

$$b_8(\theta) = -\frac{1}{889206903}(\theta - 1)^2\theta^2\left(35000000000\theta^2 - 35000000000\theta + 11250000000\right).$$

9.3. Summary of sixth order schemes

In table 5 we summarize the MIRK and CMIRK schemes of sixth order, derived in this section. For comparison purposes, we also include data for the 3-point Gauss collocation scheme in the last line of the table. We note that since its stages are implicit, the cost per subinterval associated with this scheme is generally higher than for a MIRK scheme. Since the natural interpolant for the Gauss scheme is only third order and has only C^0 continuity, we do not include data for it. However, it is possible to use the techniques considered in this paper to construct a sixth order CMIRK scheme for this Gauss scheme that gives a C^1 interpolant – see [16].

Table 5
Summary of sixth order schemes.

Type	MIRK schemes			CMIRK schemes		
	s	q	C_7	s^*	C_7	C_7'
O	6	3	0.00038	9	0.00038	0.0021
S	5	3	0.00025	8	0.00025	0.00053
S	3	3	0.00017	–	–	–

10. Numerical examples

In this section, we present two numerical examples which support the analysis provided for the optimal 5-stage, sixth order, stage order 3, symmetric MIRK scheme (15) and its associated CMIRK scheme (16). Our analysis indicates that they should provide significant improvements over the MIRK/CMIRK pair currently implemented in MIRKDC.

The first test problem (TP1) is a simple nonlinear problem [27]

$$y''(t) = \frac{3}{2}y^2(t), \qquad y(0) = 4, \qquad y(1) = 1, \tag{17}$$

which is perhaps somewhat unusual in that, despite its simple form, there are two distinct solutions; the simpler of these is $y(t) = 4/(1+t)^2$. The second test problem (TP2) is a nonlinear fluid flow problem [1]

$$\varepsilon f''''(t) = -f(t)f'''(t) - g(t)g'(t), \qquad \varepsilon g''(t) = f'(t)g(t) - f(t)g'(t), \tag{18}$$

with boundary conditions

$$f(0) = f(1) = f'(0) = f'(1) = 0, \qquad g(0) = -1, \qquad g(1) = 1.$$

For this test, $\varepsilon = 0.01$. This problem does not have a closed form solution. For each problem, an initial guess for the solution is obtained from a straight line approximation through the boundary conditions.

We modified several subroutines in MIRKDC so that the new MIRK and CMIRK schemes were available under the "methods" option for the code. The MIRKDC software computes and controls a estimate of the relative defect in the continuous approximate solution, $u(t)$, given by

$$\text{defect}(t) = \frac{|u'(t) - f(t, u(t))|}{1 + |f(t, u(t))|}. \tag{19}$$

Defect estimates are obtained by MIRKDC by sampling (19) at several points on each subinterval of the current mesh. Since it is (19) which is central to the behavior of the MIRKDC code – the defect estimates are used for both a termination criterion and for mesh selection – we focus our numerical testing on it.

Our first test involves examining the accuracy of the defect of the approximate solutions computed by MIRKDC using (i) the original MIRK/CMIRK pair and (ii) the new MIRK/CMIRK pair (15), (16) to solve (17) and (18). We consider uniform meshes of 2^m subintervals, for $m = 2, \ldots, 6$ and report the maximum value of the relative defect (19) of the computed solution, obtained by sampling it at 100 001 uniformly distributed points over the problem interval. The computation is set up so that MIRKDC computes the approximate solution on the given mesh, constructs the interpolant, estimates the defect, and then terminates. In all tests, the estimated defect obtained by MIRKDC was within a factor of 2 or 3 of the actual defect. (See [14] for further discussion.) The results for (17) are given in table 6 and the results for (18) are given in table 7.

For a given mesh, the approximate solution obtained using MIRKDC with the new MIRK/CMIRK pair has a substantially smaller defect than that obtained using

Table 6
Comparison of defects of approximate solutions, (TP1).

Pair	Number of subintervals				
	4	8	16	32	64
(i)	1.2×10^{-3}	2.4×10^{-5}	4.1×10^{-7}	6.9×10^{-9}	1.1×10^{-10}
(ii)	3.0×10^{-5}	6.5×10^{-7}	1.2×10^{-8}	2.1×10^{-10}	3.4×10^{-12}

Table 7
Comparison of defects of approximate solutions, (TP2).

Pair	Number of subintervals				
	4	8	16	32	64
(i)	1.1×10^{-1}	8.1×10^{-3}	3.8×10^{-4}	1.3×10^{-5}	3.6×10^{-7}
(ii)	2.4×10^{-2}	6.0×10^{-4}	1.9×10^{-5}	4.8×10^{-7}	1.0×10^{-8}

MIRKDC with the original pair; the defect values reported for the new pair are usually about 7% of those of the original pair or less.

Our second test involves examining the impact of the new MIRK/CMIRK pair over a complete run of the MIRKDC software. That is, MIRKDC will begin with a coarse mesh and a desired defect tolerance, and then proceed through a sequence of steps, each of which involves setting up and solving a discrete system, and then using the defect estimates for the approximate solution to determine a new mesh for the next step. (See [15] for a more detailed description of the algorithm upon which MIRKDC is based.) We will use MIRKDC to solve (17) and (18) to within a defect tolerance of 10^{-9}, beginning with a uniform mesh of 2 subintervals, and report on the performance obtained using the original and new pairs. The results are given in tables 8 and 9. For each pair we report Nsub, the number of subintervals in each mesh generated by MIRKDC as well as the corresponding defect estimate, Def Est. The final row reports the actual defect for each final approximate solution.

From tables 8 and 9, we see that the improved interpolant leads to better defect estimates which in turn enhance the ability of the code to determine a suitable final mesh, more quickly and using fewer mesh points. Similar improved performance was observed in earlier testing of the MIRKDC code when 1-point and 2-point defect sampling were investigated [14].

Table 8
Comparison of MIRKDC execution sequences, (TP1).

Pair (i)		Pair (ii)	
Nsub	Def Est	Nsub	Def Est
2	5.3×10^{-2}	2	9.7×10^{-4}
8	9.0×10^{-6}	8	2.6×10^{-7}
32	1.1×10^{-9}	20	5.1×10^{-10}
40	2.0×10^{-10}		
Actual	2.0×10^{-10}	Actual	5.3×10^{-10}

Table 9
Comparison of MIRKDC execution sequences, (TP2).

Pair (i)		Pair (ii)	
Nsub	Def Est	Nsub	Def Est
2	2.5×10^{1}	2	3.1×10^{0}
4	9.8×10^{-2}	4	1.7×10^{-2}
16	4.3×10^{-4}	16	2.3×10^{-6}
64	5.4×10^{-8}	58	2.2×10^{-9}
107	5.3×10^{-10}	69	3.0×10^{-10}
Actual	5.3×10^{-10}	Actual	6.3×10^{-10}

11. Summary and conclusions

In this paper several optimization criteria are identified and applied in the derivation of optimal MIRK and CMIRK schemes of orders 1–6. In table 10, we summarize the results. Recall that the order of the schemes is p; for each MIRK scheme, the *Type* of the scheme is either symmetric (S) or one-sided (O), the number of stages is s, the stage order is q; for each CMIRK scheme within which the MIRK scheme is embedded, the number of stages is s^*. All the symmetric schemes are A-stable. All the one-sided schemes are L-stable.

- For even order, it is possible to derive symmetric MIRK schemes of maximum stage order that achieve the lower bounds for number of stages required, as reported in [4]. However, the requirements for one-sidedness and maximum stage order sometimes force the MIRK schemes to use more than the minimum number of stages, usually 1 or 2 extra stages. In either case, except for low order, it is usually possible to embed the MIRK scheme in a CMIRK scheme which employs the minimum number of extra stages.
- The C_{p+1} values are all usually reasonably small, with those of the higher order schemes being smaller than those of the lower order scheme, and the ratios, C_{p+2}/C_{p+1}, are usually in the range 1.0–2.0. The corresponding C_{p+1} values for the CMIRK schemes, within which these MIRK schemes are embedded, are sometimes larger but usually by at most a factor of 2.

Table 10
Summary of derived MIRK and CMIRK schemes.

p	MIRK schemes				CMIRK schemes		
	Type	s	q	C_{p+1}	s^*	C_{p+1}	C'_{p+1}
1	O	1	1	0.50	2	0.50	0.75
2	O	2	2	0.017	3	0.017	0.025
2	S	1	1	0.093	3	0.093	0.14
2	S	2	2	0.12	2	0.12	0.18
3	O	2	2	0.024	3	0.024	0.043
3	O	4	3	0.048	4	0.048	0.085
4	O	5	3	0.00030	5	0.00085	0.0052
4	S	3	3	0.0057	4	0.0057	0.0090
4	S	4	3	0.0048	4	0.0048	0.010
4	S	2	2	0.0043	–	–	–
5	O	5	3	0.0012	6	0.0012	0.0022
5	O	3	3	0.0010	–	–	–
6	O	6	3	0.00038	9	0.00038	0.0021
6	S	5	3	0.00025	8	0.00025	0.00053
6	S	3	3	0.00017	–	–	–

- It is frequently possible to increase the stage order of a scheme to the maximum possible by using one extra stage. However, the higher stage order scheme often has a C_{p+1} value that is somewhat larger than that of the lower stage order scheme.
- The 3-stage, fourth order, stage order 3, symmetric MIRK scheme is optimal among 3-stage, symmetric, MIRK schemes. On the other hand, the CMIRK scheme within which it is embedded in MIRKDC is not optimal. We have shown that it is possible to derive a new CMIRK scheme with a C_5' value that is approximately 10% smaller.
- We have derived a 5-stage, sixth order, stage order 3, symmetric, MIRK scheme whose C_7 value is approximately 8% smaller than that of the more widely known MIRK scheme of this type. In addition, we have derived a new CMIRK scheme, containing this optimal MIRK scheme, which improves upon the one currently implemented in MIRKDC. The new CMIRK scheme uses one less stage and has a C_7 value that is about 90% smaller. The numerical examples suggest that these new sixth order schemes can have a substantial impact on the efficiency of the MIRKDC code.

Acknowledgements

The author would like to thank Kerri Bowers, Debra MacLean, and Isaac Muloloni for their assistance with the programming aspects of this work. The author would like to acknowledge the many helpful suggestions of the referees.

Appendix A

A.1. A 4-stage, fourth order, symmetric, MIRK scheme

In this subsection we consider 4-stage MIRK schemes in an attempt to derive a fourth order, stage order 3, symmetric, MIRK scheme which has a C_5 value that is smaller than that reported for the optimal 3-stage, fourth order, stage order 3, symmetric, MIRK scheme [2]. The general form for the tableau of a 4-stage symmetric MIRK scheme is

$$\begin{array}{c|c|cccc} c_1 & c_1 & 0 & 0 & 0 & 0 \\ 1-c_1 & 1-c_1 & 0 & 0 & 0 & 0 \\ c_3 & v_3 & x_{31} & x_{32} & 0 & 0 \\ 1-c_3 & 1-v_3 & -x_{32} & -x_{31} & 0 & 0 \\ \hline & & b_1 & b_1 & b_3 & b_3 \end{array}.$$

We impose the maximum stage order of 3 and apply the order conditions for order 4. This gives a one parameter family with SOV $= (4,4,3,3)$ and with free parameter $c_3 \neq 0,1$. Analysis of C_5 shows that we have a minimum value of $C_5 \approx 0.0048$ when $c_3 = \frac{1}{2} \pm \sqrt{5}/10$. Then $C_6 \approx 0.0082$ and $C_6/C_5 \approx 1.7$. This C_5 value is approximately 20% smaller than that of the 3-point Lobatto scheme. The tableau is

$$\begin{array}{c|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 \\
\frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{1}{2}-\frac{7\sqrt{5}}{50} & \frac{1}{10}+\frac{\sqrt{5}}{50} & \frac{-1}{10}+\frac{\sqrt{5}}{50} & 0 & 0 \\
\frac{1}{2}+\frac{\sqrt{5}}{10} & \frac{1}{2}+\frac{7\sqrt{5}}{50} & \frac{1}{10}-\frac{\sqrt{5}}{50} & \frac{-1}{10}-\frac{\sqrt{5}}{50} & 0 & 0 \\
\hline
 & & \frac{1}{12} & \frac{1}{12} & \frac{5}{12} & \frac{5}{12}
\end{array},$$

and the stability function is

$$R(z)=\frac{1+\frac{1}{2}z+\frac{1}{12}z^2}{1-\frac{1}{2}z+\frac{1}{12}z^2}.$$

This scheme is easily embedded in a 4-stage, fourth order, stage order 3, CMIRK scheme. The result is a special case of the fourth order CMIRK family given in [22]. The SOV $=(4,4,3,3)$, $C_5 \approx 0.0048$, $C_6 \approx 0.0082$, $C_6/C_5 \approx 1.7$, $C_5' \approx 0.010$, $C_6' \approx 0.017$, and $C_6'/C_5' \approx 1.7$. The tableau of the resultant CMIRK scheme is

$$\begin{array}{c|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 \\
\frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{1}{2}-\frac{7\sqrt{5}}{50} & \frac{1}{10}+\frac{\sqrt{5}}{50} & \frac{-1}{10}+\frac{\sqrt{5}}{50} & 0 & 0 \\
\frac{1}{2}+\frac{\sqrt{5}}{10} & \frac{1}{2}+\frac{7\sqrt{5}}{50} & \frac{1}{10}-\frac{\sqrt{5}}{50} & \frac{-1}{10}-\frac{\sqrt{5}}{50} & 0 & 0 \\
\hline
 & & b_1(\theta) & b_1(\theta) & b_3(\theta) & b_3(\theta)
\end{array},$$

where

$$b_1(\theta)=-\frac{1}{12}\theta\left(15\theta^3-4\theta^2+36\theta-12\right), \qquad b_2(\theta)=\frac{1}{12}\theta^2\left(15\theta^2-20\theta+6\right),$$

$$b_3(\theta)=\frac{\sqrt{5}}{12}\theta^2\left(15\theta^2-\left(30+2\sqrt{5}\right)\theta+15+3\sqrt{5}\right),$$

$$b_4(\theta)=-\frac{\sqrt{5}}{12}\theta^2\left(15\theta^2-\left(30-2\sqrt{5}\right)\theta+15-3\sqrt{5}\right).$$

These weight polynomials, which were determined using the continuous order conditions for fourth order, also satisfy the continuity conditions (6).

A.2. A 5-stage, sixth order, MIRK scheme

We consider the 5-stage, sixth order, stage order 3, MIRK family of [4] further. The family has two free parameters, c_3 and c_4. We then ask if it is possible to use the free parameters to impose extra stage order on the third, fourth, or fifth stages (without considering one-sidedness or symmetry). It is easily shown that it is impossible to impose stage order 4 on the third stage. Application of the stage order 4 condition to either the fourth or fifth stages leads to the requirement that $c_4=\frac{1}{2}\pm\sqrt{5}/10$ (and then c_5 becomes $\frac{1}{2}\mp\sqrt{5}/10$). With this choice of c_4 both the fourth and fifth stages have stage order 4 and $b_3=0$. Attempting to impose stage order 5 on either the fourth or fifth stage leads to the requirement that $c_3=\frac{1}{2}+\sqrt{5}/25\pm\sqrt{5}\sqrt{29}/50$. With this choice of c_3 both the fourth and fifth stages satisfy the stage order 5 conditions. Thus we have a pair of 5 stage, sixth order, MIRK schemes with SOV $= (6,6,3,5,5)$. The tableau of one of these schemes is

$$\begin{array}{c|c|ccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2}+\frac{\sqrt{5}}{25}+\frac{\sqrt{5}\sqrt{29}}{50} & \frac{1}{2}+\frac{142\sqrt{5}}{3125}+\frac{167\sqrt{5}\sqrt{29}}{6250} & x_{31} & x_{32} & 0 & 0 & 0 \\
\frac{1}{2}+\frac{\sqrt{5}}{10} & \frac{1}{2}+\frac{23\sqrt{5}}{250}+\frac{3\sqrt{5}\sqrt{29}}{125} & x_{41} & x_{42} & x_{43} & 0 & 0 \\
\frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{1}{2}+\frac{37\sqrt{5}}{250}-\frac{3\sqrt{5}\sqrt{29}}{125} & x_{51} & x_{52} & x_{53} & x_{54} & 0 \\
\hline
 & & \frac{1}{12} & \frac{1}{12} & 0 & \frac{5}{12} & \frac{5}{12}
\end{array},$$

where

$$x_{31} = \frac{23}{250} - \frac{17\sqrt{5}}{6250} - \frac{\sqrt{29}}{250} - \frac{21\sqrt{5}\sqrt{29}}{6250},$$
$$x_{32} = \frac{-23}{250} - \frac{17\sqrt{5}}{6250} + \frac{\sqrt{29}}{250} - \frac{21\sqrt{5}\sqrt{29}}{6250},$$
$$x_{41} = \frac{17}{400} - \frac{9\sqrt{5}}{2000} - \frac{\sqrt{29}}{400} - \frac{3\sqrt{5}\sqrt{29}}{2000},$$
$$x_{42} = \frac{-17}{400} - \frac{9\sqrt{5}}{2000} + \frac{\sqrt{29}}{400} - \frac{3\sqrt{5}\sqrt{29}}{2000}, \qquad x_{43} = \frac{17\sqrt{5}}{1000} - \frac{21\sqrt{5}\sqrt{29}}{1000},$$
$$x_{51} = \frac{23}{400} - \frac{31\sqrt{5}}{2000} + \frac{\sqrt{29}}{400} + \frac{3\sqrt{5}\sqrt{29}}{2000},$$
$$x_{52} = \frac{-23}{400} - \frac{31\sqrt{5}}{2000} - \frac{\sqrt{29}}{400} + \frac{3\sqrt{5}\sqrt{29}}{2000},$$
$$x_{53} = \frac{-17\sqrt{5}}{1000} + \frac{21\sqrt{5}\sqrt{29}}{1000}, \qquad x_{54} = \frac{-\sqrt{5}}{5}.$$

The stability function is $R(z) = P(z)/Q(z)$, where

$$P(z) = \left(\frac{-1}{600} - \frac{\sqrt{5}-\sqrt{29}}{1200}\right)z^4 + \left(\frac{-1}{600} - \frac{\sqrt{5}}{100} + \frac{\sqrt{29}}{200}\right)z^3 + \left(\frac{2}{25} - \frac{\sqrt{5}}{20} + \frac{\sqrt{29}}{100}\right)z^2 + \left(\frac{1}{2} - \frac{\sqrt{5}}{10}\right)z + 1$$

and

$$Q(z) = \left(\frac{-1}{600} + \frac{\sqrt{5}+\sqrt{29}}{1200}\right)z^4 + \left(\frac{1}{600} - \frac{\sqrt{5}}{100} - \frac{\sqrt{29}}{200}\right)z^3 + \left(\frac{2}{25} + \frac{\sqrt{5}}{20} + \frac{\sqrt{29}}{100}\right)z^2 - \left(\frac{1}{2} + \frac{\sqrt{5}}{10}\right)z + 1.$$

This scheme is A-stable and has $C_7 \approx 0.00024$, $C_8 \approx 0.00053$, and $C_8/C_7 \approx 2.2$.

A.3. A 9-stage, sixth order, CMIRK family

We derive a 9-stage, sixth order, CMIRK family which contains the optimal 6-stage, sixth order, one-sided, MIRK scheme (14) embedded within it. The extra stages will all be required to have stage order 6; thus this CMIRK family will have the SOV $= (6, 6, 3, 3, 4, 4, 6, 6, 6)$. A sixth order scheme, with stage order 3, must satisfy six order conditions of the form

$$b(\theta)^T c^{p-1} = \frac{1}{p}\theta^p, \quad p = 1, \ldots, 6, \tag{A.1}$$

and four other conditions which, after applying an elimination step, can be rewritten as

$$b(\theta)^T\left(Xc^3 + \frac{v}{4} - \frac{c^4}{4}\right) = 0, \qquad b(\theta)^T c\left(Xc^3 + \frac{v}{4} - \frac{c^4}{4}\right) = 0, \tag{A.2}$$

$$b(\theta)^T\left(Xc^4 + \frac{v}{5} - \frac{c^5}{5}\right) = 0, \qquad b(\theta)^T X\left(Xc^3 + \frac{v}{4} - \frac{c^4}{4}\right) = 0. \tag{A.3}$$

Since all but the third and fourth stages satisfy the stage order 5 conditions, $Xc^3 + v/4 - c^4/4$, the vector of stage order 4 conditions, has nonzeros only in its third and fourth positions. The two equations in (A.2) reduce to

$$b_3(\theta) = -b_4(\theta) \quad \text{and} \quad b_3(\theta) = -3b_4(\theta) \quad \Rightarrow \quad b_3(\theta) = b_4(\theta) \equiv 0.$$

Since all but the third, fourth, fifth, and sixth stages satisfy the stage order 6 conditions, $Xc^4 + v/5 - c^5/5$, the vector of stage order 5 conditions, has nonzeros only in its third through sixth positions. The first of the equations in (A.3) reduces to

$$b_5(\theta) = b_6(\theta).$$

With these substitutions, and an examination of the components of the vector, $X(Xc^3 + v/4 - c^4/4)$, it can be seen that the second equation of (A.3) reduces to

$$(x_{73} + x_{74})b_7(\theta) + (x_{83} + x_{84})b_8(\theta) + (x_{93} + x_{94})b_9(\theta) = 0,$$

which can be satisfied for all $b_7(\theta)$, $b_8(\theta)$, $b_9(\theta)$, provided

$$x_{73} = -x_{74}, \qquad x_{83} = -x_{84}, \qquad x_{93} = -x_{94}.$$

These represent extra conditions that will be imposed on the last three stages in addition to the stage order conditions. We are then left with the remaining six order conditions, (A.1), which can be used to determine the six weight polynomials $b_1(\theta)$, $b_2(\theta)$, $b_6(\theta)$, $b_7(\theta)$, $b_8(\theta)$, and $b_9(\theta)$. We have v_7, x_{71}, c_8, v_8, c_9, v_9, and x_{91} left as free parameters.

A.4. An 8-stage, sixth order, CMIRK family

Here we present a derivation which leads to an 8-stage, sixth order CMIRK family which contains the optimal 5-stage, sixth order, symmetric, MIRK scheme (15) embedded within it. We will impose stage order 5 on the sixth stage and stage order 6 on the seventh and eighth stages; the CMIRK family will have a SOV $= (6, 6, 3, 3, 3, 5, 6, 6)$. In order for this scheme to be sixth order it must satisfy the order conditions (A.1)–(A.3). Since all but the third, fourth, and fifth stages satisfy the stage order 5 conditions, $Xc^3 + v/4 - c^4/4$, the vector of stage order 4 conditions, and $Xc^4 + v/5 - c^5/5$, the vector of stage order 5 conditions, have nonzeros only in the third, fourth, and fifth positions. Consequently, the two equations (A.2) and the first equation of (A.3) reduce to ones involving only the weight polynomials $b_3(\theta)$, $b_4(\theta)$, and $b_5(\theta)$. It turns out to be possible to simultaneously satisfy these equations by solving for $b_3(\theta)$ and $b_4(\theta)$ in terms of $b_5(\theta)$:

$$b_3(\theta) = b_4(\theta) = \frac{49}{64} b_5(\theta).$$

With these substitutions, and an examination of the components of the vector $X(Xc^3 + v/4 - c^4/4)$, it can be seen that the second equation of (A.3) reduces to

$$\sum_{r=6}^{8} \left(x_{r5} - \frac{32}{49}(x_{r3} + x_{r4}) \right) b_r(\theta) = 0,$$

which can be satisfied for all $b_6(\theta)$, $b_7(\theta)$, $b_8(\theta)$, provided

$$x_{r5} = \frac{32}{49}(x_{r3} + x_{r4}), \quad r = 6, \ldots, 8.$$

These represent extra conditions that will be imposed on the last three stages in addition to the stage order conditions. This leaves the remaining six order conditions to determine the six weight polynomials $b_1(\theta)$, $b_2(\theta)$, $b_5(\theta)$, $b_6(\theta)$, $b_7(\theta)$, and $b_8(\theta)$. We have v_6, v_7, c_8, and v_8 left as free parameters.

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