Symmetric Runge-Kutta Methods with Higher Derivatives and Quadratic Extrapolation^{*}

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Abstract. In this paper we study the symmetry of Runge-Kutta methods with higher derivatives. We find conditions which provide this property for the above numerical methods. We prove that the family of E-methods constructed earlier consists of symmetric methods only, which lead to the quadratic extrapolation technique in practice.

1 Introduction

Here, we study Runge-Kutta methods with higher derivatives applied to ordinary differential equations (ODEs) of the form

$$x'(t) = g(t, x(t)), \quad t \in [t_0, t_0 + T], \quad x(t_0) = x^0 \quad (1)$$

where $x(t) \in \mathbb{R}^n$ and $g : D \subset \mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$ is a sufficiently smooth function. We remark that these numerical methods proved their efficiency. So, there are many papers published in this field (see [2], [3], [5], [7], [8], [11], [12], [13] and so on).

All methods of such sort can be represented as follows:

$$x_{ki} = x_k + \tau_k \sum_{j=1}^l \sum_{r=0}^{p_j} \tau_k^r a_{ij}^{(r)} g^{(r)}(t_{kj}, x_{kj}), \quad i = 1, 2, \dots, l, \quad (2a)$$

$$x_{k+1} = x_k + \tau_k \sum_{j=1}^l \sum_{r=0}^{p_j} \tau_k^r b_j^{(r)} g^{(r)}(t_{kj}, x_{kj}), \quad k = 0, 1, \dots, K-1, \quad (2b)$$

where $x_0 = x^0$, $t_{kj} \stackrel{\text{def}}{=} t_k + c_j \tau_k$, $g^{(r)}(t_{kj}, x_{kj})$ denotes the r -th derivative¹ of the right-hand side of problem (1) with respect to t evaluated at the point (t_{kj}, x_{kj}) ,

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¹ Here and below the zero-derivative implies the original function.

the coefficients $a_{ij}^{(r)}$, $b_j^{(r)}$ and c_j , $i, j = 1, 2, \dots, l$, $r = 0, 1, \dots, p_j$ are real numbers ($c_j \in [0, 1]$), and τ_k is a step size which may be fixed or variable. In general, the numbers p_j of the used derivatives are not equal.

When method (2) is implicit the important task is its correct implementation. In this case, we have to involve an additional iterative scheme and to keep a sufficient number of iteration steps, as indicated in [11], [12], in order to ensure high order convergence rate.

Here, we investigate the symmetry property of method (2). We find the conditions on the coefficients $a_{ij}^{(r)}$, $b_j^{(r)}$ and c_j which guarantee that method (2) is symmetric. For example, these conditions are used to prove the symmetry of E-methods developed in [11], [12]. Actually, the present study extends the results given in [4], [9] and [10] to the class of Runge-Kutta methods with higher derivatives. We just want to emphasize that symmetric numerical methods are of great importance when applied to reversible problems (see [6]) or when used as underlying methods in extrapolation algorithms (see the cited papers). However, we restrict ourselves to the quadratic extrapolation issue only in this paper.

2 Symmetric Runge-Kutta Methods with Higher Derivatives

It is clear that any particular Runge-Kutta method (2) with higher derivatives is determined uniquely by the set of coefficients $a_{ij}^{(r)}$, $b_j^{(r)}$ and c_j . Therefore, following Butcher's idea (see, for example, [1] or [4]), we represent method (2) by a partitioned tableau of the form

$$\begin{array}{c|ccccccc}
 c_1 & a_{11}^{(0)} & a_{11}^{(1)} & \dots & a_{11}^{(p_1)} & \dots & a_{1l}^{(0)} & a_{1l}^{(1)} & \dots & a_{1l}^{(p_l)} \\
 c_2 & a_{21}^{(0)} & a_{21}^{(1)} & \dots & a_{21}^{(p_1)} & \dots & a_{2l}^{(0)} & a_{2l}^{(1)} & \dots & a_{2l}^{(p_l)} \\
 \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
 c_l & a_{l1}^{(0)} & a_{l1}^{(1)} & \dots & a_{l1}^{(p_1)} & \dots & a_{ll}^{(0)} & a_{ll}^{(1)} & \dots & a_{ll}^{(p_l)} \\
 \hline
 & b_1^{(0)} & b_1^{(1)} & \dots & b_1^{(p_1)} & \dots & b_l^{(0)} & b_l^{(1)} & \dots & b_l^{(p_l)}
 \end{array} \tag{3}$$

containing all the coefficients of a Runge-Kutta method with higher derivatives. The matrix A , consisting of the coefficients $a_{ij}^{(r)}$, is a real matrix of dimension $l \times (p_1 + p_2 + \dots + p_l)l$, and the other coefficients form the real vectors b and c of dimensions $(p_1 + p_2 + \dots + p_l)l$ and l , respectively, in tableau (3).

It is known that symmetric one-step methods are defined via their adjoint counterparts, as explained, for example, in [4, p. 219–222] or in [9]. Therefore our task now is to extend the appropriate results derived for coefficients of adjoint Runge-Kutta methods to the case of method (2) involving higher derivatives.

So, we start with

Theorem 1. *Let method (2) be an l -stage Runge-Kutta formula with higher derivatives, whose coefficients are given by tableau (3). Then its adjoint method*

is equivalent to an l -stage Runge-Kutta formula with higher derivatives of the form (2) whose coefficients $a_{ij}^{(r)-}$, $b_j^{(r)-}$ and c_j^- satisfy

$$c_j^- = 1 - c_{l+1-j}, \quad (4a)$$

$$a_{ij}^{(r)-} = (-1)^r (b_{l+1-j}^{(r)} - a_{l+1-i, l+1-j}^{(r)}), \quad (4b)$$

$$b_j^{(r)-} = (-1)^r b_{l+1-j}^{(r)}, \quad r = 0, 1, \dots, p_j, \quad i, j = 1, 2, \dots, l. \quad (4c)$$

Proof. It is well-known (see the cited papers) that in order to find the adjoint Runge-Kutta method with higher derivatives we have to interchange the pair (t_k, x_k) with the pair (t_{k+1}, x_{k+1}) and to replace τ with $-\tau$ in the increment function of the method (2). It follows from the fact that method (2) belongs to the class of one-step methods.

Having fulfilled this transformation we arrive at an l -stage Runge-Kutta method of the form

$$x_{ki} = x_k + \tau_k \sum_{j=1}^l \sum_{r=0}^{p_j} (-1)^r \tau_k^r (b_j^{(r)} - a_{ij}^{(r)}) g^{(r)}(t_{kj}, x_{kj}), \quad i = 1, 2, \dots, l, \quad (5a)$$

$$x_{k+1} = x_k + \tau_k \sum_{j=1}^l \sum_{r=0}^{p_j} (-1)^r \tau_k^r b_j^{(r)} g^{(r)}(t_{kj}, x_{kj}), \quad k = 0, 1, \dots, K-1, \quad (5b)$$

where $t_{kj} = t_k + (1 - c_j)\tau_k$. If we now rearrange the nodes $c_i^- = 1 - c_{l+1-i}$ of method (5) to make them increasing; i.e., rearrange indexes by the rule $i \longleftrightarrow l+1-i$ and $j \longleftrightarrow l+1-j$ we will yield the conventional Runge-Kutta method with higher derivatives of the form (2) whose coefficients $a_{ij}^{(r)-}$, $b_j^{(r)-}$ and c_j^- satisfy formulas (4). The theorem is proved.

Papers [4, p. 219–222], [9] define a symmetric one-step method to be a method whose increment function coincides with the increment function of its adjoint method. Thus, Theorem 1 says that it is sufficient to require the following equalities:

$$c_j = 1 - c_{l+1-j}, \quad (6a)$$

$$a_{ij}^{(r)} = (-1)^r (b_{l+1-j}^{(r)} - a_{l+1-i, l+1-j}^{(r)}), \quad (6b)$$

$$b_j^{(r)} = (-1)^r b_{l+1-j}^{(r)}, \quad r = 0, 1, \dots, p_j, \quad i, j = 1, 2, \dots, l. \quad (6c)$$

Note that formulas (6) will be necessary for the symmetry if method (2) is irreducible (see [14]). It is also important to understand that conditions (6b), (6c) imply

$$p_j = p_{l+1-j}, \quad j = 1, 2, \dots, l; \quad (7)$$

i.e., equality (7) is required for any symmetric irreducible Runge-Kutta method with higher derivatives.

Our next goal is to show that symmetric irreducible Runge-Kutta methods of the form (2) do exist.

3 Symmetry of E-Methods with Higher Derivatives

To approach this, we refer to the family of Runge-Kutta methods with higher derivatives constructed by the collocation technique with multiple nodes (see [11], [12]). They have been called E-methods with higher derivatives and are of the form

$$x_{k+1/2} = x_k + \tau_k \sum_{r=0}^p \tau_k^r \left(a_1^{(r)} g_k^{(r)} + a_3^{(r)} g_{k+1}^{(r)} \right) + \tau_k a_2^{(0)} g_{k+1/2}^{(0)}, \quad (8a)$$

$$x_{k+1} = x_k + \tau_k \sum_{r=0}^p \tau_k^r \left(b_1^{(r)} g_k^{(r)} + b_3^{(r)} g_{k+1}^{(r)} \right) + \tau_k b_2^{(0)} g_{k+1/2}^{(0)} \quad (8b)$$

where $g_{k+i}^{(r)} \stackrel{\text{def}}{=} g^{(r)}(t_{k+i}, x_{k+i})$, $i = 0, 1/2, 1$, and p is the number of derivatives of the right-hand side of problem (1) used to compute the numerical solution. Evidently, method (8) belongs to the class of Runge-Kutta methods with higher derivatives, and its coefficients form the tableau

$$\begin{array}{c|cccccccc} 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ 1/2 & a_1^{(0)} & a_1^{(1)} & \dots & a_1^{(p)} & a_2^{(0)} & a_3^{(0)} & a_3^{(1)} & \dots & a_3^{(p)} \\ 1 & b_1^{(0)} & b_1^{(1)} & \dots & b_1^{(p)} & b_2^{(0)} & b_3^{(0)} & b_3^{(1)} & \dots & b_3^{(p)} \\ \hline & b_1^{(0)} & b_1^{(1)} & \dots & b_1^{(p)} & b_2^{(0)} & b_3^{(0)} & b_3^{(1)} & \dots & b_3^{(p)} \end{array} \quad (9)$$

and satisfy

$$\begin{aligned} a_1^{(r)} &= \frac{p+1}{r!2^{p+r+2}} \sum_{i=0}^{p-r} \sum_{l=0}^{i+r} \sum_{j=0}^{p+1} \frac{(-1)^l (i+r)!}{l!(i+r-l)!j!(p+1-j)!(l+j+2)} \\ &\times \sum_{q=0}^i \frac{(p+q)!}{q!2^q}, \quad r = 0, 1, \dots, p, \end{aligned} \quad (10a)$$

$$a_2^{(0)} = \frac{(p+1)!}{2} \sum_{l=0}^{p+1} \frac{(-1)^l}{l!(p+1-l)!(2l+1)}, \quad (10b)$$

$$\begin{aligned} a_3^{(r)} &= \frac{(-1)^{r+1}(p+1)}{r!2^{p+r+2}} \sum_{i=0}^{p-r} \sum_{l=0}^{i+r} \sum_{j=0}^{p+1} \frac{(-1)^j (i+r)!}{l!(i+r-l)!j!(p+1-j)!(l+j+2)} \\ &\times \sum_{q=0}^i \frac{(p+q)!}{q!2^q}, \quad r = 0, 1, \dots, p, \end{aligned} \quad (10c)$$

$$b_1^{(r)} = a_1^{(r)} + (-1)^r a_3^{(r)}, \quad b_2^{(0)} = 2a_2^{(0)}, \quad b_3^{(r)} = (-1)^r a_1^{(r)} + a_3^{(r)}. \quad (10d)$$

It was proven in [12] that method (8) with the coefficients calculated by formulas (10) is A -stable for any p . Thus, the E-methods with higher derivatives are a good means for a practical implementation when differentiation of the right-hand side of ODE (1) is not too complicated. Now we prove the symmetry of method (8).

Theorem 2. *E-method (8) with coefficients (10) is symmetric for any integer $p \geq 0$.*

Proof. To prove this theorem, it is sufficient to check the symmetry conditions (6), (7) for the coefficients in tableau (9) satisfying formulas (10) (see Section 2). It is obvious that (6a) and (7) hold. Then, by calculating the right-hand side of formula (6b) applied to the method (8) and using (10d), we obtain the following:

$$\begin{aligned} (-1)^r (b_3^{(r)} - a_3^{(r)}) &= (-1)^r ((-1)^r a_1^{(r)} + a_3^{(r)} - a_3^{(r)}) = a_1^{(r)}, \\ (-1)^r (b_2^{(0)} - a_2^{(0)}) &= (-1)^r ((-1)^r a_2^{(0)} + a_2^{(0)} - a_2^{(0)}) = a_2^{(0)}, \\ (-1)^r (b_1^{(r)} - a_1^{(r)}) &= (-1)^r ((-1)^r a_3^{(r)} + a_1^{(r)} - a_1^{(r)}) = a_3^{(r)}. \end{aligned}$$

The condition (6b) also holds. In the same way, we easily check the last condition (6c). Theorem 2 is proved.

Next, we confirm this theoretical result with the numerical examples below which show that method (8) with coefficients (10) provide quadratic extrapolation for different values of the parameter p . We refer the reader to [4], [10] for particulars of quadratic extrapolation.

4 Quadratic Extrapolation

First, we apply formulas (10) to calculate coefficients of the following E-methods of orders 6 and 8, respectively; i.e., when $p = 1$ and $p = 2$:

$$x_{k+1/2} = x_k + \frac{131}{480} \tau_k g_k^{(0)} + \frac{23}{960} \tau_k^2 g_k^{(1)} - \frac{19}{480} \tau_k g_{k+1}^{(0)} + \frac{7}{960} \tau_k^2 g_{k+1}^{(1)} + \frac{4}{15} \tau_k g_{k+1/2}^{(0)}, \quad (11a)$$

$$x_{k+1} = x_k + \frac{7}{30} \tau_k (g_k^{(0)} + g_{k+1}^{(0)}) + \frac{1}{60} \tau_k^2 (g_k^{(1)} - g_{k+1}^{(1)}) + \frac{8}{15} \tau_k g_{k+1/2}^{(0)}; \quad (11b)$$

$$\begin{aligned} x_{k+1/2} &= x_k + \frac{689}{2240} \tau_k g_k^{(0)} + \frac{169}{4480} \tau_k^2 g_k^{(1)} + \frac{17}{8960} \tau_k^3 g_k^{(2)} - \frac{81}{2240} \tau_k g_{k+1}^{(0)} \\ &\quad + \frac{41}{4480} \tau_k^2 g_{k+1}^{(1)} - \frac{19}{26880} \tau_k^3 g_{k+1}^{(2)} + \frac{8}{35} \tau_k g_{k+1/2}^{(0)}, \end{aligned} \quad (12a)$$

$$\begin{aligned} x_{k+1} &= x_k + \frac{57}{210} \tau_k (g_k^{(0)} + g_{k+1}^{(0)}) + \frac{1}{35} \tau_k^2 (g_k^{(1)} - g_{k+1}^{(1)}) \\ &\quad + \frac{1}{840} \tau_k^3 (g_k^{(2)} + g_{k+1}^{(2)}) + \frac{16}{35} \tau_k g_{k+1/2}^{(0)}. \end{aligned} \quad (12b)$$

Second, we test E-methods (11) and (12) on the problem

$$x'_1(t) = 2t x_2(t)^{1/5} x_4(t), \quad x'_2(t) = 10t \exp\{5(x_3(t) - 1)\} x_4(t), \quad (13a)$$

$$x'_3(t) = 2t x_4(t), \quad x'_4(t) = -2t \ln\{x_1(t)\} \quad (13b)$$

where $x_i(0) = 1$, $i = 1, 2, 3, 4$. Problem (13) has the following exact solution:

$$x_1(t) = \exp\{\sin(t^2)\}, \quad x_2(t) = \exp\{5 \sin(t^2)\}, \quad x_3(t) = \sin(t^2) + 1, \quad x_4(t) = \cos(t^2).$$

Table 1. Global errors of the E-method (11) with q extrapolations applied to (13)

q	fixed step size				
	$\tau = 1.00 \cdot 10^{-1}$	$\tau = 6.67 \cdot 10^{-2}$	$\tau = 4.44 \cdot 10^{-2}$	$\tau = 2.96 \cdot 10^{-2}$	$\tau = 1.98 \cdot 10^{-2}$
0	$1.1822 \cdot 10^{-01}$	$1.2221 \cdot 10^{-02}$	$1.0970 \cdot 10^{-03}$	$9.6250 \cdot 10^{-05}$	$8.4474 \cdot 10^{-06}$
1	$1.3139 \cdot 10^{-04}$	$4.1088 \cdot 10^{-06}$	$1.2647 \cdot 10^{-07}$	$5.1884 \cdot 10^{-09}$	$2.1093 \cdot 10^{-10}$
2	$1.8188 \cdot 10^{-06}$	$1.4897 \cdot 10^{-08}$	$2.0497 \cdot 10^{-10}$	$3.9575 \cdot 10^{-12}$	$3.6386 \cdot 10^{-13}$

Table 2. Global errors of the E-method (12) with q extrapolations applied to (13)

q	fixed step size				
	$\tau = 1.00 \cdot 10^{-1}$	$\tau = 6.67 \cdot 10^{-2}$	$\tau = 4.44 \cdot 10^{-2}$	$\tau = 2.96 \cdot 10^{-2}$	$\tau = 1.98 \cdot 10^{-2}$
0	$2.2594 \cdot 10^{-03}$	$7.9717 \cdot 10^{-05}$	$2.9465 \cdot 10^{-06}$	$1.1041 \cdot 10^{-07}$	$4.4174 \cdot 10^{-09}$
1	$3.1320 \cdot 10^{-06}$	$2.8233 \cdot 10^{-08}$	$3.1639 \cdot 10^{-10}$	$6.1941 \cdot 10^{-12}$	$2.4070 \cdot 10^{-13}$
2	$2.2455 \cdot 10^{-08}$	$5.6611 \cdot 10^{-11}$	$6.6482 \cdot 10^{-13}$	$3.5671 \cdot 10^{-13}$	$1.4103 \cdot 10^{-13}$

Our aim in this section is to check that E-methods (11) and (12) are symmetric and, in fact, provide quadratic extrapolation in practice. To do this, we perform numerical integrations of problem (13) with 5 different fixed step sizes $\tau_k = \tau$ on the interval $[0, 3]$, as indicated in Tables 1 and 2. We use these methods without extrapolation ($q = 0$), with one extrapolation step ($q = 1$) and with two extrapolations ($q = 2$) as well. However, the underlying methods are implicit. Therefore we apply the Newton iteration with the trivial predictor in order to obtain the required numerical solution and keep the number of iteration steps per grid point high enough to ensure that the extrapolation works properly (see [10] for more detail). We choose integers 1,2,3 and so on as the extrapolation sequence. The exact solution mentioned above is used to calculate the global errors of the integrations in the sup-norm and, hence, to find the actual order of the extrapolation algorithms.

Tables 1 and 2 exhibit clearly that the quadratic extrapolation definitely works with E-methods (11) and (12); i.e., each step of the extrapolation algorithm raises the accuracy of the underlying method by two orders. This experiment confirms also that both E-methods are symmetric and the theoretical results given above are correct.

5 Conclusion

In this paper we have discussed the symmetry property of Runge-Kutta methods with higher derivatives. We have found the coefficients of adjoint Runge-Kutta methods with higher derivatives (Theorem 1) and determined the general conditions on the coefficients of the methods under consideration to be symmetric (formulas (6), (7)). The new result is an extension of the well-known formulas for conventional Runge-Kutta methods (see the cited papers) and, of course, covers this case. Finally, we have given some examples of symmetric Runge-Kutta

methods with higher derivatives and confirmed this property with practical computations. From this point of view, the family of E-methods derived earlier in [11] and [12] looks attractive if the cost of the derivative calculation is not too high. However, more experiments are needed to identify practical properties of the E-methods in detail.

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