

Improved Starting Methods for Two-Step Runge–Kutta Methods of Stage-Order $p - 3$

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Abstract.

In [5], Jackiewicz and Verner derived formulas for, and tested the implementation of two-step Runge-Kutta (TSRK) pairs. For pairs of orders 3 and 4, the error estimator accurately tracked the exact local truncation error on several nonlinear test problems. However, for pairs designed to achieve order 8, the results appeared to be only of order 6.

This deficiency was identified in [2] by Hairer and Wanner who used B-series to formulate a complete set of order conditions for TSRK methods, and showed that if the order of a TSRK method is at least two greater than its stage-order, special starting values are necessary for the first step.

In [8], Verner showed that such starting values have to be perturbed from their asymptotically correct values to include errors of precisely the form which the selected TSRK formula is designed to propagate from step to step. It was shown that starting values could be obtained by solving the problem using a complementary set of Runge–Kutta methods which satisfied perturbed order conditions to obtain perturbed starting values, and that such methods could be obtained by solving these order conditions directly. The design used there required solving an intricate polynomial equation. Here, the design is improved, and new starting methods are simpler to derive, and perhaps may lead to starting methods for TSRK methods of order 8.

Key words. two-step Runge–Kutta methods, starting methods, order conditions, local error estimation, implementation.

AMS subject classifications. 65L05, 65L06, 65L20.

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1 Introduction

A variety of types of explicit step by step methods for approximating solutions to an initial value differential problem

$$\begin{cases} y'(x) = f(y(x)), & x \in [x_0, x_{end}], \\ y(x_0) = y_0, \end{cases} \quad (1)$$

are known. In this article, we assume continuity of $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ that is sufficient to guarantee a unique solution, and study improvements to the *implementation* of a subset of explicit two-step Runge–Kutta (TSRK) methods designed by Jackiewicz and Tracogna [4]. Such TSRK methods use s past derivative with the current solution approximations to propagate the solution from step to step in an attempt to reduce the number (s) of new derivative values per step from that required by a similar standard Runge–Kutta method. The restricted subset considered may be formulated as

$$\begin{cases} Y_i^j = y_i + h \sum_{k=1}^s \left(a_{jk} f(Y_{i-1}^k) + b_{jk} f(Y_i^k) \right), \\ y_{i+1} = y_i + h \sum_{k=1}^s \left(v_k f(Y_{i-1}^k) + w_k f(Y_i^k) \right), \end{cases} \quad (2)$$

$j = 1, 2, \dots, s$, and for each $i = 1, 2, \dots, N-1$, solutions y_i are propagated over N steps of fixed size $h = (x_{end} - x_0)/N$. The coefficients in (2) are selected so that Taylor expansions of the approximation satisfy $y_i = y(x_i) + O(h^p)$, and the internal stage approximations Y_i to $y(x_i + c_j h)$ for $x_i = x_0 + ih$ satisfy $\{Y_i^j = y(x_i + c_j h) + O(h^{\min(q+1, p)})\}$, $j = 1, \dots, s$, for a selected order p and stage-order $q \leq p$.

On comparison of these approximate with the exact solutions, these constraints lead to algebraic *order* conditions which are conveniently written as matrix equations in terms of a Butcher tableau written with a vector $\mathbf{c} = (A + B)\mathbf{e}$ as

$$\frac{\mathbf{c}}{v^T} \left| \begin{array}{c|c} A & B \\ \hline v^T & w^T \end{array} \right. = \begin{array}{c|cccc|cc} c_1 & a_{11} & a_{12} & \dots & a_{1s} & & \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} & b_{21} & \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} & b_{s1} & \dots & b_{s,s-1} \\ \hline & v_1 & v_2 & \dots & v_s & w_1 & w_2 & \dots & w_s \end{array} \quad (3)$$

Table 1: A TSRK as a Butcher tableau

We restrict attention to methods with B a lower triangular matrix, so that the approximations are defined explicitly, and the order conditions up to $p=6$ satisfied have been tabulated by Jackiewicz and Tracogna [4] using matrices A and B , the diagonal matrix C with $\mathbf{c}=C\mathbf{e}$ where $\mathbf{e}=[1, 1, \dots, 1]^t$ and vector \mathbf{c} . Pairs of TSRK methods were derived by solving these order conditions directly, and some pairs are included in [5].

Failure of an order 8 pair to manifest the design order in several test problems led to a more precise study of the expected approximations which revealed that exact starting values in the initial step were inadequate to launch a correct propagation. Rather, TSRK methods are designed to propagate stage values Y_0^j , $j = 1, \dots, s$ of order $q \leq p$ for which the terms of orders $q + 1, \dots, p - 1$ have a structure which is preserved in all succeeding steps. This is clearly demonstrated in [8], and there it was suggested in the spirit of Runge–Kutta methods of "effective order" developed by Butcher [1], that the problem could be overcome by constructing special starting methods for the first step. There, we showed how to derive one type of starting method for a TSRK method of order 6 and stage-order 3.

To begin propagation using (2), we require an initial solution y_0 (which can be selected as the initial value $y(x_0)$, stage values Y_0^j , $j = 1, \dots, s$, for the first step, and y_1 , an approximation to $y(x_0 + h)$). In [8], we proposed that these initial stage values be obtained by s Runge–Kutta methods specially designed to yield correctly *perturbed* asymptotic values in place of the exact stage values. For the case studied with $p=6$, and $q=3$, four Runge–Kutta methods with *seven* stages each were designed and derived in terms of arbitrary nodes. The choice to use seven stages was based on the assumption that these methods would behave like RK methods of order 6. Unfortunately, this provided surplus freedom in the choice of arbitrary parameters, and in the ensuing derivation, it was necessary to solve a substantial and non-obvious polynomial for one of the nodes. The value y_1 was obtained from a standard Runge–Kutta method of order 6.

While this strategy succeeded for TSRK methods of order 6, a subsequent attempt to apply this strategy to obtaining starting methods for a TSRK of order 8 failed. Accordingly, we devised a new design for starting TSRK methods of order 6 which uses a set of Runge–Kutta starting methods each having only *six* stages. This considerably simplifies the derivation, and yields an alternate procedure for deriving starting methods.

To begin the derivation, we obtain a TSRK method of order p , satisfying the order conditions (eg. tabulated up to order 6 by Jackiewicz and Tracogna [4]), for example by the direct solution approach developed in [5]. These standard order conditions depend on (scalar) quadrature expressions

$$Q^{[k]} = \frac{1}{(k-1)!} \left(v^T (C - I)^{k-1} + w^T C^{k-1} - \frac{1}{k} \right) \mathbf{e}, \quad (4)$$

$k = 1, 2, \dots, p$, and the (vector) subquadrature expressions

$$\tilde{C}^{[k]} = \frac{1}{(k-1)!} \left(A(C - I)^{k-1} + BC^{k-1} - \frac{C^k}{k} \right) \mathbf{e}. \quad (5)$$

In particular, for a method of order p and stage-order q , $Q^{[k]} = 0$, $k = 1, \dots, p$ and $\tilde{C}^{[k]} = 0$, $k = 1, \dots, q$. These two sets of order conditions are linear in v, w and A, B respectively, and easily solved for restricted subsets of these parameters. The remaining conditions take the form $M\tilde{C}^{[k]} = 0$ or a linear combination of these for $q < k < p$ with M being a product of $v^t + w^t$ or v^t with up to $p - k - 1$ factors of $A, A + B, C$, and these may be solved using the remaining arbitrary parameters.

When $q < p - 1$, conditions of the latter type are required, so it becomes necessary to perturb the starting values Y_0^j . This perturbation may be executed by using a set of Runge–Kutta "starting methods" each of which satisfies perturbed order conditions. In particular, to start a TSRK method of order p and stage-order $p - 3$, each special starting method must satisfy all conditions up to order $p - 3$. Further, each standard condition of order $p - 2$ of the form $\Phi(t) = 1/\gamma(t)$ is replaced by $\Phi(t) = (1 + \hat{C}_j^{[p-2]})/\gamma(t)$; each condition of order $p - 1$ of the form $\overline{bA}\phi(\tilde{t}) = 1/\gamma(t)$, is replaced by $\overline{bA}\phi(\tilde{t}) = (1 + \hat{C}_j^{[p-1]} + A\widehat{pBC}_j^{[p-2]})/\gamma(t)$, with $\hat{C}_j^{[k]}$ and $A\widehat{pBC}_j^{[p-2]}$ defined in (6) and (7), and each remaining condition of order $p - 1$ of form $\Phi(t) = 1/\gamma(t)$ is replaced by $\Phi(t) = (1 + \hat{C}_j^{[p-1]})/\gamma(t)$. (Here, we use t to denote a rooted tree in the context developed by Butcher for order conditions.) Thus, to complement a TSRK method of order 6, each of s starting methods must satisfy these special conditions up to order $p - 1$, and for $p - 1 = 5$, these are tabulated explicitly in [8].

2 Solving the Order Conditions

We now focus on a four-stage TSRK method of stage-order 3 and order 6 with coefficients represented by $\{\mathbf{v}, \mathbf{w}, A, B, \mathbf{c}\}$. For such a method, we modify the process in [8], to obtain a set of starting Runge–Kutta methods with stage-order 2 and only six stages for each by adapting the strategy developed in [7]. We shall refer to the order conditions in Table 5 of [8] to

obtain each of the four required Runge–Kutta starting methods, and begin with an algorithm to calculate coefficients $\{\bar{\mathbf{b}}, \bar{\mathbf{A}}, \bar{\mathbf{c}}\}$. First compute

$$\hat{C}_j^{[k]} = \frac{i! \tilde{C}^{[k]}}{c_j^i}, \quad k = 4, 5, \quad j = 1, \dots, 4, \quad (6)$$

and

$$[\widehat{ApBC}^{[4]}]_j = \frac{[5!C^{-5}(A+B)\tilde{C}^{[4]}]_j}{c_j^5} \quad (7)$$

from the coefficients of the TSRK method.

Algorithm 2.1

1. Choose nodes $\bar{c}_1 = 0, \bar{c}_6 = 1, \bar{c}_2, \bar{c}_3, \bar{c}_5$ arbitrary, and then \bar{c}_4 as a zero of the polynomial

$$\begin{aligned} p(\hat{C}_j^{[4]}, \hat{C}_j^{[5]}, [\widehat{ApBC}^{[4]}]_j) = \\ \frac{\hat{C}_j^{[4]}(2\bar{c}_4 - \bar{c}_3)}{1440} \left(5\hat{C}_j^{[4]} + 3[\widehat{ApBC}^{[4]}]_j - \hat{C}_j^{[4]} + 9 \right) \\ - \frac{\hat{C}_j^{[4]}}{144} \bar{c}_3 \bar{c}_4 (2 + \bar{c}_3) + \left(\frac{[\widehat{ApBC}^{[4]}]_j}{360} + \frac{\hat{C}_j^{[5]}}{288} \right) \bar{c}_3 \bar{c}_4 \end{aligned} \quad (8)$$

2. Choose $\bar{b}_2 = 0$, and the remaining weights $\bar{b}_i, i = 1, 3, \dots, 6$ to satisfy the five linear "perturbed quadrature" conditions:

$$\begin{aligned} \bar{b}^t \bar{C}^{k-1} \mathbf{e} &= \frac{1}{k}, \quad k = 1, 2, 3, \\ &= \frac{1 + \hat{C}_j^{[k]}}{k}, \quad k = 4, 5. \end{aligned} \quad (9)$$

3. For each of $r=1, 2, 3$, choose $(\bar{b}^t \bar{A}^r)_2 = 0$, and compute the homogeneous polynomials $(\bar{b}^t \bar{A}^r)_j, j = 1, 3, \dots, 6 - r$, by solving the three linear systems

$$\begin{aligned} (\bar{b}^t \bar{A}^r) \bar{C}^{k-1} \mathbf{e} &= \frac{1}{k(k+1) \dots (k+r)}, \quad k = 1, \dots, 3 - r, \\ &= \frac{1 + \hat{C}_j^{[k+r]} + (\widehat{ApBC}^{[k+r-1]})_j}{k(k+1) \dots (k+r)}, \quad k = 4 - r, \dots, 5 - r. \end{aligned} \quad (10)$$

4. Choose $\bar{a}_{32}, \bar{a}_{42}$ and \bar{a}_{43} to satisfy

$$\bar{a}_{32}\bar{c}_2 - \frac{\bar{c}_3^2}{2}, \quad \sum_{j=3}^4 \bar{a}_{4j}\bar{c}_j - \frac{\bar{c}^2}{2} \quad (11)$$

and the equation

$$(\bar{\mathbf{b}}^t \bar{\mathbf{A}})_5 \left[\sum_{j=3}^4 \bar{b}_j(\bar{c}_j - 1)\bar{a}_{j2} \right] = \left[\bar{b}_5(\bar{c}_5 - 1) \sum_{j=3}^4 (\bar{\mathbf{b}}^t \bar{\mathbf{A}})_j \bar{a}_{j2} \right], \quad (12)$$

5. Now compute the remainder of the coefficients \bar{a}_{ij} by the backward recursion

$$\bar{a}_{7-r,j} = \frac{(\bar{\mathbf{b}}^t \bar{\mathbf{A}}^r)_j - \sum_{i=j+1}^{6-r} (\bar{\mathbf{b}}^t \bar{\mathbf{A}}^{r-1})_i \bar{a}_{ij}}{(\bar{\mathbf{b}}^t \bar{\mathbf{A}}^{r-1})_{7-r}}, \quad r = 1, 2, 3, \quad j = 6-r, \dots, 1, \quad (13)$$

This yields a three parameter family (in $\bar{c}_2, \bar{c}_3, \bar{c}_5$) of starting methods for each of the s=4 starting values needed. (These three parameters need not be the same for each of the four starting methods.) To see that the order conditions of Table 5 in [8] are satisfied, observe that (9) imply that conditions 1,2,3,5,9, hold, and (10) imply conditions 4,7,14, 8,16 and 17. Provided that they are nonzero, the homogeneous polynomials together with the stage-order conditions (11) imply that $\sum_{j=1}^{k-1} \bar{a}_{ij}\bar{c}_j - \bar{c}_i^2/2$, $i = 5, 6$. These conditions may now be used to establish conditions 4,10,11,15. Finally, (12) implies that conditions 12 and 13 hold simultaneously, and the nodal constraint (8) implies that 12 is valid. Thus, this algorithm can be used with various choices of the arbitrary parameters to select appropriate starting methods for each internal stage value Y_j^0 . In addition, a value of y_1 of order 6 is required, and this is computed with a standard Runge–Kutta method of order 6.

For experiments, we construct a TSRK method with nodes $c_1 = 1/125$, $c_2 = 2/5$, $c_3 = 13/20$, $c_4 = 1$. (It was observed in [8] that $c_1 \neq 0$ for otherwise, we cannot compute $\widehat{ApBC}^{[4]}$ which contains the factor C^{-5} , and an alternate computation is not obvious, if it is possible.) As in [8], we choose c_1 to be small in order to clearly show the pathology that is removed by starting methods, even though the weights required for c_1 for this improved starting method remain very large.

$\frac{1}{125}$	-0.1447	0.6146	-0.6435	0.1816				
$\frac{2}{5}$	-0.6413	3.0394	-3.6064	0.9583	$\frac{13}{20}$			
$\frac{13}{20}$	-0.4551	2.0730	-2.3099	0.2417	$\frac{5}{8}$	0.4752		
1	-1.0585	4.6502	-4.7586	$\frac{4}{5}$	$\frac{1}{7}$	$\frac{8}{9}$	0.3351	
	-0.8127	0.7965	-1.6680	$\frac{13}{50}$	1.7487	-1.3318	1.2675	$\frac{1}{120}$

Table 2: Approximate coefficients of a TSRK method of stage-order 3 and order 6 with nodes $c_1 = 1/125, c_2 = 2/5, c_3 = 13/20, c_4 = 1$

In [8] the author presented the results of two experiments for estimating the order of TSRK methods. In the first test, six problems (a quadrature problem $y' = 7x^6, y(0) = 1$, and problems A1, A4, B5, D1 and E3 from DETEST [3]) were solved using a fixed stepsize. Of these five were solved on the interval $[0,20]$, and Euler's problem was solved on $[0,2\pi]$. Global errors were obtained using exact or accurate endpoint values, and these were used to estimate the achieved order of accuracy p , by assuming that the global error was proportional to h^p . Results obtained when exact starting values are used give clear evidence that such an implementation of a TSRK method has only order 5. The results are not repeated here for the TSRK method selected, but are similar to the results in Table 4a of [8]. However, Table 3 shows the Taylor series expansions for two problems when accurate starting values are used. Although the leading local truncation error is a term in h^5 , this term remains identical in all succeeding propagated values, so the global error is proportional to h^5 .

Taylor series of Error for Linear Problem

Starting step:	0.00000
TSRK step 2:	$.00175 h^5 - .01222 h^6 + .00659 h^7 + O(h^8)$
TSRK step 3:	$.00175 h^5 - .00350 h^6 + .05278 h^7 + O(h^8)$

Taylor series of Error for Logistic Problem

Starting step:	0.0000
TSRK step 2:	$-.567 \cdot 10^{-6} h^5 - .797 \cdot 10^{-6} h^6 + .455 \cdot 10^{-7} h^7 + O(h^8)$
TSRK step 3:	$-.567 \cdot 10^{-6} h^5 - .162 \cdot 10^{-6} h^6 - .415 \cdot 10^{-6} h^7 + O(h^8)$

Table 3: Leading error terms in three steps of TSRK6

0						
$\frac{1}{8}$	0.125					
$\frac{3}{8}$	-0.1875	0.5625				
.1875	-0.4687	0.2812	-0.4687			
$\frac{3}{4}$	-0.1942	1.1249	1.1250	-1.4999		
1	1.7961	1.4999	4.6848	-6.7402	-0.2406	
	-4.099E10	0	1.309E11	1.344E11	5.449E10	-1.696E10

Table 4: Approximate coefficients of the starting method for node $c_1 = 1/125$

h	Quadrature Problem		Linear Problem A1		Logistic Problem A4	
	<i>ge</i>	<i>p</i>	<i>ge</i>	<i>p</i>	<i>ge</i>	<i>p</i>
0.2	.12221(10 ⁻⁴)		0.15461(10 ⁻¹⁶)		0.78828(10 ⁻¹²)	
0.2/2	0.19144(10 ⁻⁶)	5.99	0.41784(10 ⁻¹⁸)	5.20	0.13822(10 ⁻¹³)	5.83
0.2/4	0.29950(10 ⁻⁸)	5.99	0.78945(10 ⁻²⁰)	5.72	0.22775(10 ⁻¹⁵)	5.92
0.2/8	0.46827(10 ⁻¹⁰)	5.99	0.13396(10 ⁻²¹)	5.88	0.36506(10 ⁻¹⁷)	5.96
0.2/16	0.73190(10 ⁻¹²)	5.99	0.21758(10 ⁻²³)	5.94	0.57759(10 ⁻¹⁹)	5.98
0.2/32	0.11437(10 ⁻¹³)	5.99	0.34642(10 ⁻²⁵)	5.97	0.90809(10 ⁻²¹)	5.99
0.2/64	0.17872(10 ⁻¹⁵)	5.99	0.54632(10 ⁻²⁷)	5.98	0.14232(10 ⁻²²)	5.99
0.2/128	0.27917(10 ⁻¹⁷)	5.99	0.85756(10 ⁻²⁹)	5.99	0.22273(10 ⁻²⁴)	6.00
0.2/256	0.46616(10 ⁻¹⁹)	5.90	0.13430(10 ⁻³⁰)	5.99	0.34810(10 ⁻²⁶)	5.90
h	Euler's Problem B5†		Two Body Problem D1		Duffing's Problem E3	
	<i>ge</i>	<i>p</i>	<i>ge</i>	<i>p</i>	<i>ge</i>	<i>p</i>
0.2	0.45246(10 ⁻⁷)		0.18148(10 ⁻⁸)		0.34163(10 ⁻⁶)	
0.2/2	0.37306(10 ⁻⁹)	6.92	0.25227(10 ⁻¹⁰)	6.16	0.70184(10 ⁻⁸)	5.60
0.2/4	0.38778(10 ⁻¹¹)	6.58	0.37162(10 ⁻¹²)	6.08	0.18633(10 ⁻⁹)	5.23
0.2/8	0.50892(10 ⁻¹³)	6.25	0.56376(10 ⁻¹⁴)	6.04	0.34497(10 ⁻¹¹)	5.75
0.2/16	0.75200(10 ⁻¹⁵)	6.08	0.86797(10 ⁻¹⁶)	6.02	0.57845(10 ⁻¹³)	5.89
0.2/32	0.11557(10 ⁻¹⁶)	6.02	0.13462(10 ⁻¹⁷)	6.01	0.93356(10 ⁻¹⁵)	5.95
0.2/64	0.17967(10 ⁻¹⁸)	6.00	0.20957(10 ⁻¹⁹)	6.00	0.14815(10 ⁻¹⁶)	5.97
0.2/128	0.28025(10 ⁻²⁰)	6.00	0.32685(10 ⁻²¹)	6.00	0.23325(10 ⁻¹⁸)	5.98
0.2/256	0.43755(10 ⁻²²)	6.00	0.51024(10 ⁻²³)	6.00	0.36582(10 ⁻²⁰)	5.99

Table 5a. Order estimates using a fixed stepsize implementation of a new TSRK of order 6, and stage-order 3, implemented with four perturbed starting values.

To demonstrate the improvement in order numerically, we construct a set of starting methods each with the same arbitrary nodes $\bar{c}_2 = 1/8, \bar{c}_3 = 3/8, \bar{c}_5 = 3/4$, and tabulate in Table 4 approximate coefficients of the first starting method. When the six test problems are solved with fixed stepsizes, Table 5a clearly indicates that the design order 6 is achieved in practical computations. Moreover, in Table 5b, the Taylor series expansions using perturbed starting values of the new starting methods also show that order 6 is achieved algebraically for the two problems selected.

Taylor series of Error for Linear Problem	
Perturbing starting step:	$.248 \cdot 10^{-4} h^8 + O(h^9)$
TSRK step 2:	$.00557 h^7 - .02088 h^8 + O(h^9)$
TSRK step 3:	$.00648 h^7 - .02543 h^8 + O(h^9)$
Taylor series of Error for Logistic Problem	
Perturbing starting step:	$-.196 \cdot 10^{-9} h^7 + O(h^8)$
TSRK step 2:	$.297 \cdot 10^{-6} h^7 - O(h^8)$
TSRK step 3:	$.263 \cdot 10^{-6} h^7 + O(h^8)$

Table 5b: Leading error terms in three steps of TSRK6
implemented with a corrective starting method

3 Conclusions

A hope to construct valid starting methods for TSRK methods of order 8 and low stage-order motivated a study to simplify the construction of starting methods necessary for the correct implementation of TSRK methods. This led to a much improved design, and the numerical results illustrate that the new starting methods are effective. Even so, comparisons of the results in Table 5a with corresponding results for two highly efficient Runge–Kutta methods also of order 6 shows that the Runge–Kutta methods are equally efficient [8]. Because the implementation of explicit Runge–Kutta methods is considerably simpler, it appears that explicit Runge–Kutta methods will remain the method of choice for most practical problem solving. In this direction, the author constructed an improved Runge–Kutta pair of methods of orders 5 and 6 as a target method for comparison with TSRK methods, and the coefficients of this new pair appears on the author’s website.

Still, research on general linear methods remains active with a view to discovering better algorithms, and so the development here may be considered as a constructive contribution to the development and study of such

algorithms.

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