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HIGHER ORDER APPROXIMATIONS OF RUNGE-KUTTA TYPE

by E. Baylis Shanks

George C. Marshall Space Flight Center
Huntsville, Ala.

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SUMMARY

The fourth-order formula of Runge-Kutta has been used extensively to obtain approximate solutions of differential equations of first, second, and higher orders. This formula requires only four evaluations of the function involved in the differential equation while the fifth-order formula of Kutta-Nystrom requires six evaluations of the function. The sixth-order formula of Huta is not known as well, and has the disadvantage of requiring eight evaluations of the function. No formulas of higher order except those developed in this investigation seem to exist in the literature. These formulas are "self-starting" and therefore extremely useful in combination with efficient "continuing" procedures.

Formulas of higher order, including the seventh and eighth orders, are developed in this paper. Moreover, more efficient formulas requiring fewer evaluations are developed for orders five and six. All possible formulas are displayed for those orders below five.

FORMULATION OF THE PROBLEM

1. General. The differential equations considered are of the form $y' = f(x,y)$, since systems of the first and higher orders are reducible to an application of this result. The function f is assumed to be analytic in a sufficiently large neighborhood of the initial point (x_0, y_0).

Let f_i be defined by the equation

$$f_i = f(x_0 + a_i h,\ y_0 + a_i h \sum_{j=0}^{i-1} b_{ij} f_j),$$

where $f_0 = f(x_0, y_0)$ and $i = 1, 2, \ldots, n$. Consider the finite series

$$Y = y_0 + h \sum_{i=0}^{n} c_i f_i$$

The a_i, b_{ij}, c_i are parameters to be determined so that Y and the solution $y(x_0 + h)$ of the given differential equation will agree to some desired degree of accuracy.

It is immediate that a necessary and sufficient condition that the Taylor series for Y and the Taylor series for the solution $y(x_0 + h)$ of the given differential equation agree through terms in h^m is that

$$\left(f^{(k-1)}\right)_o = k \sum_{i=0}^{n} c_i \left(f_i^{(k-1)}\right)_o \tag{1}$$

for $k = 1, 2, \ldots, m$, where the symbol $f^{(k)}$ is used for the $k^{\underline{th}}$ derivative of the function $f(x_0 + h, y(x_0 + h))$.

To specify a given formula, the coefficients may be detached as follows:

	Formula
a_1	$a_1\, b_{10}$
a_2	$a_2\, b_{20} + a_2 b_{21}$
.	
.	
.	
a_n	$a_n\, b_{n0} + a_n\, b_{n1} + \ldots + a_n b_{n,n-1}$
	$c_0 + c_1 + \ldots + c_n$

This array specifies the formula

$$Y = y_0 + h \sum_{i=0}^{n} c_i f_i \ ,$$

where

$$f_o = f(x_0, y_0)$$

$$f_1 = f(x_0 + a_1 h,\ y_0 + a_1 h\, b_{10} f_0)$$

$$f_2 = f(x_0 + a_2 h,\ y_0 + a_2 h(b_{20} f_0 + b_{21} f_1)$$

$$\vdots$$

$$f_n = f(x_0 + a_n h,\ y_0 + a_n h(b_{n0} f_0 + b_{n1} f_1 + \ldots + b_{n,n-1} f_{n-1}))$$

Such arrays will be used consistently to specify such formulas.

Let $1 = \sum_{i=0}^{n} c_i$ and $1 = \sum_{j=0}^{i-1} b_{ij}$ for $i = 1, 2, \ldots, n$. Let $i_1 + 2i_2 + \ldots + ki_k = k$,

$Q^1_{it} = a_i$, and

$$Q^k_{it} = a_i^{i_1} \left(\prod_{r=1}^{i_2} 2a_i \sum_{j=1}^{i-1} b_{ij} Q^1_{jt_r} \right) \cdots \left(\prod_{r=1}^{i_k} ka_i \sum_{j=1}^{i-1} b_{ij} Q^{k-1}_{jt_r} \right) \tag{2}$$

for $k = 2, 3, \ldots, m - 1$. Finally, let

$$1 = (k + 1) \sum_{i=1}^{n} c_i Q^k_{it} \tag{3}$$

for $m \geq 2$ and $k = 1, 2, \ldots, m - 1$. These equations are sufficient conditions that the equations (1) be satisfied, giving a formula of order m, as is proved in a paper presented by the author at the summer meeting of the American Mathematical Society in Boulder, Colorado, on August 29, 1963. An abstract of this paper appears in the American Mathematical Society Notices, Volume 10, Number 5, Issue No. 69, August, 1963. The subscripts t and t_r in the Q^k_{it} are introduced to distinguish the different products for fixed i and k.

The equations (3) can now be written for each $k = 1, 2, \ldots, m - 1$ in succession. Such equations for the first two values of k are given next.

$k = 1$: $$1 = 2 \sum_{j_1=1}^{n} c_{j_1} a_{j_1}$$

$k = 2$: $$1 = 3 \sum_{j_1=1}^{n} c_{j_1} a_{j_1}^2$$

$$1 = 6 \sum_{j_2=1}^{n} c_{j_2} a_{j_2} \left(\sum_{j_1=1}^{j_2-1} b_{j_2 j_1} a_{j_1} \right)$$

In general, a simple induction establishes the facts that in each instance the indices for each b_{ij} are distinct and the second index j is summed for 1, 2, ..., i-1, there are no other changes of indices, and each b_{ij} is followed immediately by at least one a_j. Hence, without confusion, $b_{ij}\, a_j^k$ may be denoted by b^k and the summation signs and indices may be omitted, as for the first two values of k below.

$$k = 1: \qquad 1 = 2\ ca$$

$$k = 2: \qquad 1 = 3\ ca^2 \qquad 1 = 6\ cab$$

The equations (3) are completely determined when the Q_{it}^k are known. The rule for the inductive determination of the Q_{it}^k given in (2) is given below in the "summation convention" notation.

$$Q^k = a^{i_1} \left(\prod_{r=1}^{i_2} 2\ abQ' \right) \cdots \left(\prod_{r=1}^{i_k} kabQ^{k-1} \right) \tag{4}$$

Let a be multiplied by 1, 2 ab be multiplied (and summed) by each term of Q^1, ..., kab be multiplied (and summed) by each term of Q^{k-1}. Then the rule (4) states that a term of Q^k is formed by forming a product consisting of i_1 factors of the type mentioned first in the preceding sentence, i_2 factors of the type mentioned second in the preceding sentence, ..., and i_k factors of the type mentioned last in the preceding sentence, where $i_1 + 2\, i_2 + \ldots + k\, i_k = k$.

It is possible to state a rule so that the equations for a given k can be written without reference to the equations for smaller integers. Such a rule follows essentially from the following facts, which are easily proved: (1) Q^k is a product of factors, each factor of which consists of a sequence of an integer, a's, and b's, (2) in each factor of Q^k, at least one a precedes each b and at least one a follows each b, (3) in each factor of Q^k, the integer p immediately precedes $a^k b$ if and only if p - 1 is the number of a's that follow and are connected by summation to the given b, and (4) Q^k contains exactly the number k of a's. However, such a rule is not of much advantage, if any, since all equations for k = 1, 2, ..., m-1 are conditions to be satisfied to obtain a valid formula of order m.

To further simplify the notation, let

$$\sum_{i=j+1}^{n-k} c_i^{(k)}\, a_i\, b_{ij} = c_j^{(k+1)} \quad \text{for} \quad j = 1, 2, \ldots, n-k-1, \tag{5}$$

where $k = 0, 1, \ldots, m-3$ and, when convenient, $c_i^{(0)}, c_i^{(1)}, c_i^{(2)}, \ldots$ will be denoted by $c_i, c_i', c_i'', \ldots$ respectively. Among the sufficient conditions determined later are

$$1 = (j+1)(j+2)\ldots(j+k+1)\sum_{i=1}^{n-k} c_i^{(k)}\, a_i^j\,, \tag{6}$$

where $j = 1, 2, \ldots, m-k-1$ and $k = 0, 1, \ldots, m-2$.

For $m = n+1$, it is seen that $c_{n-k}^{(k)} \neq 0$ from the definition and the fact that $1 = (n+1)!\; c_1^{(n-1)}\, a_1$. Hence equations (5) determine the b_{ij} in terms of the $c_i^{(k)}$ and the a_k. Moreover, equations (6) determine the $c_i^{(k)}$ in terms of the a_i. In this case, the algebraic system is reduced to the conditions not included in equations (6), given the n free parameters a_i. For example, when $m = n+1 = 4$, there is one such condition $1 = 8\, ca^2b$ and three free parameters a_1, a_2, a_3.

A listing is given below of the Q^k for $k = 1, 2, 3, 4$. Formation of the list is made easier by separating the products of order $p+1$ of the type $pabQ^{p-1}$ from the other products of order $p+1$ as is done below.

$k = 1$:	a					
$k = 2$:	a^2			$2ab$		
$k = 3$:	a^3	$2a^2b$		$3ab^2$	$6abb$	
$k = 4$:	a^4	$2a^3b$	$3a^2b^2$	$4ab^3$	$8ab^2b$	$12abb^2$
	$6a^2bb$	$4a^2(b)(b)$		$24abbb$		

The term $4a^2(b)(b)$ is formed by the rule from $(2ab)(2ab)$ and is written in summation notation

$$4a_{i_2}^2 \left(\sum_{i_1=1}^{i_2-1} b_{i_2i_1}\, a_{i_1}\right)\left(\sum_{i_1=1}^{i_2-1} b_{i_2i_1}\, a_{i_1}\right)$$

or simply

$$4a_{i_2}^2 \left(\sum_{i_1=1}^{i_2-1} b_{i_2 i_1} a_{i_1} \right)^2 .$$

The term $6a^2bb$ is written

$$6a_{i_3}^2 \sum_{i_2=1}^{i_3-1} b_{i_3 i_2} a_{i_2} \left(\sum_{i_1=1}^{i_2-1} b_{i_2 i_1} a_{i_1} \right)$$

in summation notation.

For $k = 4$, it can be shown directly by an inductive process that the two conditions $1 = 30\ cabb$ and $1 = 40\ c'a^2b$ can be replaced by the one condition $7 = 120(cabb + c'a^2b)$ and that the resulting fifteen conditions for $k = 1, 2, 3, 4$ are necessary and sufficient for obtaining a valid formula for order 5. This was shown for $1 \le k \le 5$ (which includes the case $1 \le k \le 4$) in a paper by Huta [1]. The necessary and sufficient conditions for $1 \le k \le 6$ have been derived by the author and will be given below, although the sufficiency of the other conditions are generally enough for our purposes.

$k = 1$: $\quad 1 = 2ca$

$k = 2$: $\quad 1 = 3ca^2 \quad 1 = 6c'a$

$k = 3$: $\quad 1 = 4ca^3 \quad 1 = 12c'a^2 \quad 1 = 8ca^2b \quad 1 = 24c''a$

$k = 4$: $\quad 1 = 5ca^4 \quad 1 = 20c'a^3 \quad 1 = 15ca^2b^2 \quad 1 = 60c''a^2$

$1 = 10ca^3b \quad 1 = 20ca^2(b)(b) \quad 7 = 120(ca^2bb + c'a^2b) \quad 1 = 120c'''a$

$k = 5$: $\quad 1 = 6ca^5 \quad 1 = 30c'a^4 \quad 1 = 24ca^2b^3 \quad 1 = 120c''a^3$

$1 = 12ca^4b \quad 1 = 24ca^3(b)(b) \quad 1 = 18ca^3b^2 \quad 1 = 48ca^2b^2b$

$13 = 720ca^2(b)(bb) + 360c'a^2(b)(b) \quad 2 = 45(ca^3bb + c'a^3b)$

$1 = 360c'''a^2 \quad 1 = 36ca^2(b)(b^2) \quad 1 = 40(ca^2bb^2 + c'a^2b^2)$

$1 = 720c''''a \quad 1 = 60(ca^2bbb + c'a^2bb + c''a^2b)$

$k = 6$: $\quad 1 = 7ca^6 \quad 1 = 42c'a^5 \quad 1 = 35ca^2b^4 \quad 1 = 210c''a^4$

$1 = 14ca^5b \quad 1 = 21ca^4b^2 \quad 1 = 28(ca^4bb + c'a^4b)$

$1 = 28ca^4(b)(b) \quad 1 = 28ca^3b^3 \quad 9 = 280(ca^3b^2b + ca^2b^3b)$

$5 = 252(ca^3bb^2 + c'a^3b^2) \quad 1 = 42ca^3(b)(b^2) \quad 1 = 105ca^2b^2b^2$

$31 = 2520(ca^3bbb + c'a^3bb + c''a^3b) \quad 5 = 336ca^3(b)(bb) + 168c'a^3(b)(b)$

$19 = 1680(ca^2b^2bb + ca^2bb^2b + c'a^2b^2b) \quad 11 = 840(ca^2bb^3 + c'a^2b^3)$

$1 = 80ca^2(b)(b^2b) + 40ca^2b^2(b)(b) \quad 1 = 56ca^3(b)(b)(b)$

$1 = 168(ca^2bbb^2 + c'a^2bb^2 + c''a^2b^2) \quad 1 = 63ca^2(b^2)(b^2)$

$1 = 280(ca^2bbbb + c'a^2bbb + c''a^2bb + c'''a^2b)$

$1 = 56[ca^2(b)(bb^2) + ca^2(b^2)(bb) + c'a^2(b)(b^2)]$

$1 = 56ca^2(b)(b^3) \quad 1 = 840c'''a^3 \quad 1 = 2520c''''a^2 \quad 1 = 5040c'''''a$

$19 = 1260[2ca^2(b)(bbb) + ca^2(bb)(bb) + 2c'a^2(b)(bb) + c''a^2(b)(b)]$

This list could be extended, although the computation would be laborious. Instead, the extension of the list giving sufficient conditions is relatively easy. For $k = 5$, the two lists agree with the exception that certain formulas in the list just given should be replaced with other formulas as shown next.

$13 = 720ca^2(b)(bb) + 360c'a^2(b)(b)$	$1 = 72ca^2(b)(bb)$ $1 = 120c'a^2(b)(b)$
$2 = 45(ca^3bb + c'a^3b)$	$1 = 36ca^3bb$ $1 = 60c'a^3b$
$1 = 40(ca^2bb^2 + c'a^2b^2)$	$1 = 72ca^2bb^2$ $1 = 90c'a^2b^2$
$1 = 60(ca^2bbb + c'a^2bb + c''a^2b)$	$1 = 144ca^2bbb$ $1 = 180c'a^2bb$ $1 = 240c''a^2b$

The procedure is the same for $k = 6$ and is clear from our previous rules.

If $m = n + 1$ and $a_n = 1$, then it follows, for each i, that

$$c_i - c_i a_i = c_i' \,, \tag{7}$$

where $c_n' = 0$ is taken. In general, even though m and $n + 1$ are different integers, we may choose $a_n = 1$ and assume the validity of equations (7) for each i. Since an obvious requirement is that $m \le n + 1$, this will never lead to a contradiction per se. Under these circumstances, a great simplification occurs in the conditions for $k = 1, 2, \ldots, m-1$. Most equations involving c_i can be omitted because of equivalent equations involving c_i'. Some exceptions are equations like $1 = ca$ and $1 = 20ca^2(b)(b)$. Further important simplifications can be made by requiring some of the following conditions to be satisfied for appropriate i.

$$2\sum_{j=1}^{i-1} b_{ij}\, a_j = a_i \qquad 3\sum_{j=1}^{i-1} b_{ij}\, a_j^2 = a_i^2 \qquad 6\sum_{j=1}^{i-1} b_{ij}\, a_j \sum_{k=1}^{j-1} b_{jk}\, a_k = a_i^2$$

$$4\sum_{j=1}^{i-1} b_{ij}\, a_j^3 = a_i^3 \qquad \ldots$$

However, this will be treated in detail in the discussion of formulas for a given order.

GENERAL FORMULAS FOR ORDERS BELOW 4

The formulas in these cases are easy to derive and are simply listed below.

$m = 0$: $\quad Y = y_0$

$m = 1$: $\quad Y = y_0 + hf_0$

$m = 2$: $\quad Y = y_0 + h\,\dfrac{1}{2a_1}\,[(2a_1 - 1)\, f_0 + f_1]$

$m = 3$: 1. $Y = y_0 + h\frac{1}{4}[f_0 + (3 - 6c)f_1 + 6cf_2]$

$$f_1 = f(x_0 + \frac{2}{3}h,\ y_0 + \frac{2}{3}hf_0)$$

$$f_2 = f(x_0 + \frac{2}{3}h,\ y_0 + h\frac{1}{6c}[(4c - 1)f_0 + f_1])$$

2.
$$\begin{array}{ll} a_1 & a_1 \\ a_2 & a_2(b_{20} + b_{21}) \\ (c_0 + c_1 + c_2) & \end{array}$$

where

$$b_{21} = \frac{a_2(a_2 - a_1)}{a_1(2 - 3a_1)} \qquad b_{20} = 1 - b_{21}$$

$$c_1 = \frac{2 - 3a_2}{6a_1(a_1 - a_2)}, \qquad c_2 = \frac{2 - 3a_1}{6a_2(a_2 - a_1)}, \qquad c_0 = 1 - c_1 - c_2$$

For the last formula, we have detached the coefficients as explained previously. This will be done for subsequent formulas.

GENERAL FORMULAS FOR ORDER 4

In this case, $n = 3$ is taken which is its minimum value. Denote

$$\bar{b}_i = \sum_{j=1}^{i-1} b_{ij}\, a_j - \frac{1}{2}\, a_i \tag{8}$$

for $i = 1, 2, 3$, where $\bar{b}_1 = -\frac{1}{2}a_1$. Then three of the seven conditions may be written

$$ca\bar{b} = 0, \qquad ca^2\bar{b} = 0, \qquad c'a\bar{b} = 0.$$

As vectors in three space, c, ca, and c' are orthogonal to the non-zero vector $\overline{ab}$ and hence are linearly dependent. Thus, for $i = 1, 2, 3$

$$A\, c_i + B\, c_i a_i + C\, c_i' = 0$$

for some non-zero vector (A, B, C). Multiplying and summing in turn by a_i and a_i^2, we get

$$\frac{1}{2} A + \frac{1}{3} B + \frac{1}{6} C = 0,$$

$$\frac{1}{3} A + \frac{1}{4} B + \frac{1}{12} C = 0.$$

These equations imply, for each i,

$$c_i - c_i a_i = c_i' \quad \text{and} \quad a_3 = 1 \quad \text{since} \quad c_3 \neq 0.$$

With this information, it is not difficult to derive the complete solution for order 4.

First, $a_2 \neq 1$. Otherwise, $c_2' = 0$ and $c_1'' = c_2' a_2 b_{21} = 0$, but this contradicts the requirement that $1 = 24 c_1'' a_1$. Then there are three cases as discussed next.

1. $a_1 = a_2$. Then $1 = 6(c_1' + c_2') a_2$ and $1 = 12(c_1' + c_2') a_2^2$. Hence $a_1 = a_2 = \frac{1}{2}$ and $c_1' + c_2' = \frac{1}{3}$. Let $c_2 = 2c$. In this case, the formula is

$$\begin{array}{ll}
\frac{1}{2} & \frac{1}{2} \\[2ex]
\frac{1}{2} & \frac{1}{12c}\,[(6c - 1) + 1] \\[2ex]
1 & [0 + (1 - 6c) + 6c] \\[2ex]
 & \frac{1}{6}\,[1 + (4 - 12c) + 12c + 1]
\end{array}$$

The case $1 = 6c$ is the famous Runge-Kutta Fourth Order Formula.

2. $a_1 = 1$. Then $c_1' = 0$, $6c_2' a_2 = 1$, $12c_2' a_2^2 = 1$ and it follows that $a_2 = \frac{1}{2}$ and $c_2' = \frac{1}{3}$. Then $c_2 = \frac{1}{1 - a_2} c_2' = \frac{2}{3}$, so that $c_1 + c_3 = \frac{1}{2} - c_2 a_2 = \frac{1}{2} - \frac{1}{3} = \frac{1}{6}$. Let $f_3 = c$. In this case, the formula is

$$
\begin{array}{ll}
1 & 1 \\[2ex]
\frac{1}{2} & \frac{1}{8}(3 + 1) \\[2ex]
1 & \frac{1}{12c}[(12c - 3) + (-1) + 4] \\[2ex]
 & \frac{1}{6}[1 + (1 - 6c) + 4 + 6c]
\end{array}
$$

3. a_1, a_2, 1 are distinct. In this case,

$$c_1'' = \frac{1}{24a_1}, \qquad c_1' = \frac{1 - 2a_2}{12a_1(a_1 - a_2)}, \qquad c_2' = \frac{1 - 2a_1}{12a_2(a_2 - a_1)}$$

and the formula is

$$
\begin{array}{ll}
a_1 & a_1 \\[1ex]
a_2 & a_2(b_{20} + b_{21}) \\[1ex]
1 & (b_{30} + b_{31} + b_{32}) \\[1ex]
 & (c_0 + c_1 + c_2 + c_3),
\end{array}
$$

where

$$b_{21} = \frac{a_2 - a_1}{2a_1(1 - 2a_1)} \qquad\qquad b_{20} = \frac{3a_1 - 4a_1^2 - a_2}{2a_1(1 - 2a_1)}$$

$$b_{31} = \frac{(1 - a_1)(2 - a_1 - 5a_2 + 4a_2^2)}{2a_1(a_1 - a_2)(3 - 4a_1 - 4a_2 + 6a_1a_2)}$$

$$b_{32} = \frac{(1 - a_1)(1 - a_2)(1 - 2a_1)}{a_2(a_2 - a_1)(3 - 4a_1 - 4a_2 + 6a_1a_2)}$$

$$b_{30} = 1 - b_{31} - b_{32}$$

$$c_1 = \frac{2a_2 - 1}{12a_1(a_1 - a_2)(a_1 - 1)} \qquad c_2 = \frac{2a_1 - 1}{12a_2(a_2 - a_1)(a_2 - 1)}$$

$$c_3 = \frac{3 - 4a_1 - 4a_2 + 6a_1a_2}{12(a_1 - 1)(a_2 - 1)} \qquad c_0 = 1 - c_1 - c_2 - c_3$$

FORMULAS FOR ORDER 5

It will now be shown that the fifteen conditions for order 5 are inconsistent when $n = 4$, the minimum value.

Six of the conditions may be written

$$c\overline{ab} = ca^2\overline{b} = ca^3\overline{b} = c'\overline{ab} = c''\overline{ab} = (ca^2b + c'a^2)\overline{b} = 0 \ ,$$

where the notation (8) is used. In four space, the vectors c_j, c_ja_j, $c_ja_j^2$, c_j', c'' and $\sum_{i=j+1}^{n} c_ia_i^2b_{ij} + c_j'a_j$ for $j = 1, 2, 3, 4$ are orthogonal to the non-zero vector $\overline{ab}$. Since $c_4' = c_4'' = c_3'' = 0$ by convention, $A\,c_j + B\,c_j' + C\,c_j'' = 0$ implies $A = B = C = 0$. Hence c_j, c_j', and c_j'' are independent vectors, spanning the three space orthogonal to the space spanned by the vector $\overline{ab}$.

By a straightforward calculation, we get

$$c_ja_j = a_4c_j + (7 - 8a_4)\,c_j' - 20(1 - a_4)\,c_j''$$

$$c_ja_j^2 = a_4^2c_j + (6 - 8a_4^2)\,c_j' - 2(9 - 10a_4^2)\,c_j''$$

$$\sum_{i=j+1}^{n} c_ia_i^2b_{ij} + c_j'a_j = 2c_j' - 3c_j''$$

for $j = 1, 2, 3, 4$. From the last of these equations

$$c_4a_4^2b_{43} + c_3'a_3 = 2c_3' \ ,$$

which, since $c_4a_4b_{43} = c_3'$ and $c_3' \neq 0$, is equivalent to the condition $a_3 + a_4 = 2$. From the first two equations

$$c_3(a_3 - a_4) = (7 - 8a_4)c_3' ,$$

$$c_3(a_3^2 - a_4^2) = (6 - 8a_4^2)c_3' ,$$

from which it follows that

$$(a_3 + a_4)(7 - 8a_4)c_3' = (6 - 8a_4^2)c_3' .$$

Since $c_3' \neq 0$ and $a_3 + a_4 = 2$, it follows that $a_4 = 1$ and hence $a_3 = 1$ also. Since $c_j - c_j a_j = c_j'$, we get $c_3' = 0$, a contradiction.

This contradiction establishes the assertion that all of the conditions cannot be satisfied when $m = n + 1 = 5$.

One procedure at this point is to increase n from 4 to 5, which introduces additional parameters. This was done by Kutta, whose formula of the fifth order with six evaluations of the function contained an arithmetic error, later corrected by Nystrom.

However, it is not necessary to increase n from 4 to 5 if we adopt a new viewpoint. Instead of requiring that the conditions be satisfied, let us require only that they be approximately satisfied. In other words, if the condition is written in the form $F = 0$, then the new requirement is to be that $F = e$ for a sufficiently small e. In particular, for a given order m, the possibility will be examined that all conditions below order m are exactly satisfied, while some or all of order m are approximated.

For $m = 5$, let $a_4 = 1$, $c_i - c_i a_i = c_i'$ for $i = 1, 2, 3, 4$, and $\bar{b}_i = 0$ for $i = 2, 3, 4$. Let the conditions below order 5 be satisfied. Then $1 = 6c'a = 6cab = 3ca^2 - 3c_1a_1^2$, so that $c_1 = 0$ since $1 = 3ca^2$. Hence $c_1' = 0$. The new requirements then reduce to the following.

$$1 = 6c'a \qquad 1 = 12c'a^2 \qquad 1 - e' = 20c'a^3$$

$$1 = 2ca \qquad 1 = 24c''a \qquad 1 - e'' = 60c''a^2$$

$$1 - e''' = 120c'''a$$

where e', e'', and e''' are to be taken small. Since $c_1' = 0$, $3e' = 3 - 5a_2 - 5a_3 + 10a_2a_3$ and since $a_2 = 2b_{21}a_1 = 2\dfrac{c_1'''a_1}{c_2''a_2}$, we deduce $a_1(2 - 5a_2) = 2a_2e'' + 2e'''(a_1 - a_2)$.

To recapitulate, there are six parameters e', e'', e''', a_1, a_2, a_3 and five requirements, namely e', e'', e''' are to be taken small and

$$3e' = 3 - 5(a_2 + a_3) + 10a_2a_3 ,$$

$$a_1(2 - 5a_2) = 2a_2e'' + 2e'''(a_1 - a_2) .$$

When these requirements are met, a valid formula may be obtained.

The formula just developed is given by the following schema.

$$\begin{array}{ll}
a_1 & a_1 \\
a_2 & a_2(b_{20} + b_{21}) \\
a_3 & a_3(b_{30} + b_{31} + b_{32}) \\
1 & (b_{40} + b_{41} + b_{42} + b_{43}) \\
 & (c_0 + c_1 + c_2 + c_3 + c_4)
\end{array}$$

where

$$\sum_{i=j+1}^{4} c_i^{(k)} a_i b_{ij} = c_j^{(k+1)}$$

for $j = 1, 2, \ldots, 3-k$ and $k = 0, 1, 2$; $b_{i0} = 1 - b_{i1} - \ldots - b_{i,i-1}$ for $i = 2, 3, 4$; and

$$c_1''' = \frac{1 - e'''}{120 a_1}$$

$$c_1'' = \frac{-2e' + 2 - 5a_2}{120 a_1(a_1 - a_2)} \qquad c_2'' = \frac{-2e'' + 2 - 5a_1}{120 a_2(a_2 - a_1)}$$

$$c_1' = 0 \qquad c_2' = \frac{1 - 2a_3}{12 a_2(a_2 - a_3)} \qquad c_3' = \frac{1 - 2a_2}{12 a_3(a_3 - a_2)}$$

$$c_1 = 0 \qquad c_2 = \frac{1 - 2a_3}{12 a_2 (1 - a_2)(a_2 - a_3)} \qquad c_3 = \frac{1 - 2a_2}{12 a_3 (1 - a_3)(a_3 - a_2)}$$

$$c_0 = 1 - c_1 - c_2 - c_3$$

$$3e' = 3 - 5(a_2 + a_3) + 10 a_2 a_3$$

$$a_1(2 - 5a_2) = 2a_2 e'' + 2e'''(a_1 - a_2)$$

e', e'', e''' sufficiently small.

It is clear that the requirements can be satisfied and that the schema defines a four parameter set of valid formulas of the fifth order with only five evaluations. Each such formula does not qualify in the traditional sense to be called a fifth order formula, but does qualify as a fifth order formula from the new viewpoint and from a practical standpoint. Specific formulas for this and other cases are given in a later section.

FORMULAS FOR ORDER 6

In this case, let $a_5 = 1$, $c_i - c_i a_i = c_i'$ for $i = 1, 2, 3, 4, 5$, and $\bar{b}_i = 0$ for $i = 2, 3, 4, 5$. Let the conditions below order 6 be satisfied. Then $1 = 120c'''a = 120c''ab = 60c''a^2 - 60c_1''a_1^2$, so that $c_1'' = 0$ since $1 = 60c''a^2$. Similarly, $c_1' = c_1 = 0$. The new requirements then reduce to the following.

$$1 = 6c'a \qquad 1 = 12c'a^2 \qquad 1 = 20c'a^3 \qquad i - e' = 30c'a^4$$

$$1 = 24c''a \qquad 1 = 60c''a^2 \qquad i - e'' = 120c''a^3$$

$$1 = 120c'''a \qquad i - e''' = 360c'''a^2$$

$$i - e'''' = 720c''''a$$

$$1 = 2ca \qquad 1 - e = 180c'a^2bb \qquad 1 - d = 90c'a^2b^2 ,$$

where $d, e, e', e'', e''', e''''$ are to be taken small.

Since $c_1' = c_1'' = 0$, it follows that

$$\begin{aligned} 2e' &= 2 - 3(a_2 + a_3 + a_4) + 5(a_2a_3 + a_2a_4 + a_3a_4) - 10a_2a_3a_4 \\ e'' &= 1 - 2(a_2 + a_3) + 5a_2a_3. \end{aligned} \tag{9}$$

Since $a_2 = 2b_{21}a_1 = \frac{c_1''''a_1}{c_2'''a_2}$, it follows that

$$a_1(1 - 3a_2) = e'''a_2 - e''''(a_2 - a_1). \tag{10}$$

Laborious calculation leads to the following results.

$$1 - 180c'a^2bb = \frac{(1 - a_4)(1 - 5a_2) + e''''(3 - 5a_2 - 5a_4 + 10a_2a_4)}{2(2 - 5a_2)}$$

$$1 - 90c'a^2b^2 = \frac{(1 - a_4)(2 - 10a_2 + 15a_1a_2) + 2e'''(3 - 5a_2 - 5a_4 + 10a_2a_4)}{4(2 - 5a_2)} .$$

From the equations (9), we get

$$1 - a_4 = \frac{2e' + e''}{3 - 5a_2 - 5a_3 + 10a_2a_3} ,$$

which implies $1 - a_4$, $1 - 180c'a^2bb$, and $1 - 90c'a^2b^2$ are small provided e', e'', e''', e'''' are small. Hence equations $1 - e = 180c'a^2bb$ and $1 - d = 90c'a^2b^2$ will be satisfied in the presence of the other requirements.

The formula just developed is given by the following schema.

a_1	a_1
a_2	$a_2(b_{20} + b_{21})$
a_3	$a_3(b_{30} + b_{31} + b_{32})$
a_4	$a_4(b_{40} + b_{41} + b_{42} + b_{43})$
1	$(b_{50} + b_{51} + b_{52} + b_{53} + b_{54})$

$$(c_0 + c_1 + c_2 + c_3 + c_4 + c_5)$$

where

$$\sum_{i=j+1}^{5} c_i^{(k)} a_i b_{ij} = c_j^{(k+1)}$$

for $j = 1, 2, \ldots, 4-k$ and $k = 0, 1, 2, 3$; $b_{i0} = 1 - b_{i1} - \ldots - b_{i,\, i-1}$ for $i = 2, 3, 4, 5$; and

$$c_1'''' = \frac{1 - e''''}{720a_1}$$

$$c_1''' = \frac{1 - e''' - 3a_2}{360a_1(a_1 - a_2)} \qquad c_2''' = \frac{1 - e''' - 3a_1}{360a_2(a_2 - a_1)}$$

$$c_1'' = 0 \qquad c_2'' = \frac{2 - 5a_3}{120a_2(a_2 - a_3)} \qquad c_3'' = \frac{2 - 5a_2}{120a_3(a_3 - a_2)}$$

$$c_1' = 0 \qquad c_2' = \frac{3 - 5a_3 - 5a_4 + 10a_3a_4}{60a_2(a_2 - a_3)(a_2 - a_4)} \quad c_3' = \frac{3 - 5a_2 - 5a_4 + 10a_2a_4}{60a_3(a_3 - a_2)(a_3 - a_4)} \quad c_4' = \frac{3-5a_2-5a_3+10a_2a_3}{60a_4(a_4-a_2)(a_4-a_3)}$$

$$c_1 = 0 \qquad c_2 = \frac{3 - 5a_3 - 5a_4 + 10a_3a_4}{60a_2(1 - a_2)(a_2 - a_3)(a_2 - a_4)} \qquad c_3 = \frac{3 - 5a_2 - 5a_4 + 10a_2a_4}{60a_3(1 - a_3)(a_3 - a_2)(a_3 - a_4)}$$

$$c_4 = \frac{3 - 5a_2 - 5a_3 + 10a_2a_3}{60a_4(1 - a_4)(a_4 - a_2)(a_4 - a_3)}$$

$$c_5 = \frac{1}{2} - c_2a_2 - c_3a_3 - c_4a_4 \qquad c_0 = 1 - c_2 - c_3 - c_4 - c_5$$

$$2e' = 2 - 3(a_2 + a_3 + a_4) + 5(a_2a_3 + a_2a_4 + a_3a_4) - 10a_2a_3a_4$$

$$e'' = 1 - 2(a_2 + a_3) + 5a_2a_3$$

$$a_1(1 - 3a_2) = e'''a_2 - e''''(a_2 - a_1)$$

e', e'', e''', e'''' sufficiently small

It is clear that the requirements can be satisfied and that the schema defines a five parameter set of valid formulas of the sixth order with only six evaluations (in the sense of the new viewpoint).

EFFICIENT FORMULAS THROUGH ORDER 8

Using the principles already explained, we have derived other formulas. To avoid going into details and to conserve space, we will simply list a spectrum of such formulas, including formulas of the seventh and eighth orders.

Formula (4-4)

$$\begin{array}{ll}
\frac{1}{100} & \frac{1}{100} \\[2ex]
\frac{3}{5} & \frac{1}{245}\,(-4278 + 4425) \\[2ex]
1 & \frac{1}{8791}\,(524746 - 532125 + 16170) \\[2ex]
 & \frac{1}{70092}\,(-179124 + 200000 + 40425 + 8791)
\end{array} \qquad (11)'$$

Formula (5-5)

$$\begin{array}{ll}
\frac{1}{9000} & \frac{1}{9000} \\[2ex]
\frac{3}{10} & \frac{1}{10}\,(-4047 + 4050) \\[2ex]
\frac{3}{4} & \frac{1}{8}\,(20241 - 20250 + 15) \\[2ex]
1 & \frac{1}{81}\,(-931041 + 931500 - 490 + 112) \\[2ex]
 & \frac{1}{1134}\,(105 + 0 + 500 + 448 + 81)
\end{array} \qquad (12)$$

Formula (6-6)

$$\begin{array}{ll}
\frac{1}{300} & \frac{1}{300} \\[2ex]
\frac{1}{5} & \frac{1}{5}(-29 + 30) \\[2ex]
\frac{3}{5} & \frac{1}{5}(323 - 330 + 10) \\[2ex]
\frac{14}{15} & \frac{1}{810}(-510104 + 521640 - 12705 + 1925) \\[2ex]
1 & \frac{1}{77}(-417923 + 427350 - 10605 + 1309 - 54) \\[2ex]
\multicolumn{2}{l}{\frac{1}{3696}(198 + 0 + 1225 + 1540 + 810 - 77)}
\end{array} \tag{13}$$

Formula (7-7)

$$\begin{array}{ll}
\frac{1}{192} & \frac{1}{192} \\[2ex]
\frac{1}{6} & \frac{1}{6}(-15 + 16) \\[2ex]
\frac{1}{2} & \frac{1}{186}(4867 - 5072 + 298) \\[2ex]
1 & \frac{1}{31}(-19995 + 20896 - 1025 + 155) \\[2ex]
\frac{5}{6} & \frac{1}{5022}(-469805 + 490960 - 22736 + 5580 + 186) \\[2ex]
1 & \frac{1}{2604}(914314 - 955136 + 47983 - 6510 - 558 + 2511) \\[2ex]
\multicolumn{2}{l}{\frac{1}{300}(14 + 0 + 81 + 110 + 0 + 81 + 14)}
\end{array} \tag{14}$$

Formula (7-9)

$$
\begin{array}{ll}
\frac{2}{9} & \frac{2}{9} \\[2ex]
\frac{1}{3} & \frac{1}{12}(1+3) \\[2ex]
\frac{1}{2} & \frac{1}{8}(1+0+3) \\[2ex]
\frac{1}{6} & \frac{1}{216}(23+0+21-8) \\[2ex]
\frac{8}{9} & \frac{1}{729}(-4136+0-13584+5264+13104) \\[2ex]
\frac{1}{9} & \frac{1}{151632}(105131+0+302016-107744-284256+1701) \\[2ex]
\frac{5}{6} & \frac{1}{1375920}(-775229+0-2770950+1735136+2547216+81891+328536) \\[2ex]
1 & \frac{1}{251888}(23569+0-122304-20384+695520-99873-466560+241920) \\[2ex]
 & \frac{1}{2140320}(110201+0+0+767936+635040-59049-59049+635040+110201)
\end{array}
\tag{15}
$$

Formula (8-10)

$$
\begin{array}{ll}
\frac{4}{27} & \frac{4}{27} \\[2ex]
\frac{2}{9} & \frac{1}{18}(1+3) \\[2ex]
\frac{1}{3} & \frac{1}{12}(1+0+3) \\[2ex]
\frac{1}{2} & \frac{1}{8}(1+0+0+3) \\[2ex]
\frac{2}{3} & \frac{1}{54}(13+0-27+42+8)
\end{array}
\tag{16}
$$

$\frac{1}{6}$	$\frac{1}{4320}(389 + 0 - 54 + 966 - 824 + 243)$	
1	$\frac{1}{20}(-231 + 0 + 81 - 1164 + 656 - 122 + 800)$	
$\frac{5}{6}$	$\frac{1}{288}(-127 + 0 + 18 - 678 + 456 - 9 + 576 + 4)$	(16) (Cont'd)
1	$\frac{1}{820}(1481 + 0 - 81 + 7104 - 3376 + 72 - 5040 - 60 + 720)$	

$$\frac{1}{840}(41 + 0 + 0 + 27 + 272 + 27 + 216 + 0 + 216 + 41)$$

Formula (8-12)

$\frac{1}{9}$	$\frac{1}{9}$	
$\frac{1}{6}$	$\frac{1}{24}(1 + 3)$	
$\frac{1}{4}$	$\frac{1}{16}(1 + 0 + 3)$	
$\frac{1}{10}$	$\frac{1}{500}(29 + 0 + 33 - 12)$	
$\frac{1}{6}$	$\frac{1}{972}(33 + 0 + 0 + 4 + 125)$	(17)
$\frac{1}{2}$	$\frac{1}{36}(-21 + 0 + 0 + 76 + 125 - 162)$	
$\frac{2}{3}$	$\frac{1}{243}(-30 + 0 + 0 - 32 + 125 + 0 + 99)$	
$\frac{1}{3}$	$\frac{1}{324}(1175 + 0 + 0 - 3456 - 6250 + 8424 + 242 - 27)$	
$\frac{5}{6}$	$\frac{1}{324}(293 + 0 + 0 - 852 - 1375 + 1836 - 118 + 162 + 324)$	

$\frac{5}{6}$ $\quad \frac{1}{1620}(1303 + 0 + 0 - 4260 - 6875 + 9990 + 1030 + 0 + 0 + 162)$

1 $\quad \frac{1}{4428}(-8595 + 0 + 0 + 30720 + 48750 - 66096 + 378 - 729 - 1944 - 1296 + 3240)$

$$\frac{1}{840}(41 + 0 + 0 + 0 + 0 + 216 + 272 + 27 + 27 + 36 + 180 + 41) \tag{17}$$

(Cont'd)

Formulas (11), (15), and (17) have the orders indicated in the traditional sense while formulas (12), (13), (14), and (16) have the orders indicated from the new viewpoint and only for certain values of h.

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