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An Explicit Sixth-Order Runge-Kutta Formula

By H. A. Luther

1. Introduction. The system of ordinary differential equations considered has the form

$$dy/dx = f(x, y)\,, \qquad y(x_0) = y_0\,. \tag{1}$$

Here $y(x)$ and $f(x, y)$ are vector-valued functions

$$y(x) = (y_1(x), y_2(x), \cdots, y_m(x))\,,$$
$$f(x, y) = (f_1(x, y), f_2(x, y), \cdots, f_m(x, y))\,,$$

so that we are dealing with m simultaneous first-order equations.

For the fifth-order case, explicit Runge-Kutta formulas have been found whose remainder, while of order six when y is present in (1), does become of order seven when f is a function of x alone [3], [4]. This is due to the use of six functional substitutions, a necessary feature when y occurs nontrivially [1].

A family of explicit sixth-order formulas has been described [1]. In this family is the formula given in the next section. Its remainder, while of order seven when y is present in (1), is of order eight when f is a function of x alone. Here again the possibility arises because seven functional substitutions are used, rather than six. Once more, this is a necessity [2].

For selected equations (those not strongly dependent on y) such formulas seem to lead to some increase in accuracy.

2. Presentation of the Formula. For the interval $[x_n, x_n + h]$, Lobatto quadrature points leading to a remainder of order eight are

$$x_n, \qquad x_n + h/2, \qquad x_n + (7 - (21)^{1/2})h/14, \qquad x_n + (7 + (21)^{1/2})h/14, \qquad x_n + h.$$

A set of Runge-Kutta formulas related thereto is given below. They can be verified by substitution in the relations given by Butcher [1].

Expressed in a usual form they are

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$$\begin{aligned}
y_{n+1} &= y_n + \{9k_1 + 64k_3 + 49k_5 + 49k_6 + 9k_7\}/180 \\
k_1 &= hf(x_n, y_n) \\
k_2 &= hf(x_n + \nu h, y_n + \nu k_1) \\
k_3 &= hf(x_n + h/2, y_n + \{(4\nu - 1)k_1 + k_2\}/(8\nu)) \\
k_4 &= hf(x_n + 2h/3, y_n + \{(10\nu - 2)k_1 + 2k_2 + 8\nu k_3\}/(27\nu)) \\
k_5 &= hf(x_n + (7 + (21)^{1/2})h/14, y_n + \{-([77\nu - 56] + [17\nu - 8](21)^{1/2})k_1 \\
&\qquad - 8(7 + (21)^{1/2})k_2 + 48(7 + (21)^{1/2})\nu k_3 \\
&\qquad - 3(21 + (21)^{1/2})\nu k_4\}/(392\nu)) \\
k_6 &= hf(x_n + (7 - (21)^{1/2})h/14, y_n + \{-5([287\nu - 56] - [59\nu - 8](21)^{1/2})k_1 \\
&\qquad - 40(7 - (21)^{1/2})k_2 + 320(21)^{1/2}\nu k_3 + 3(21 - 121(21)^{1/2})\nu k_4 \\
&\qquad + 392(6 - (21)^{1/2})\nu k_5\}/(1960\nu)) \\
k_7 &= hf(x_n + h, y_n + \{15([30\nu - 8] - [7\nu(21)^{1/2}])k_1 + 120k_2 \\
&\qquad - 40(5 + 7(21)^{1/2})\nu k_3 + 63(2 + 3(21)^{1/2})\nu k_4 \\
&\qquad - 14(49 - 9(21)^{1/2})\nu k_5 + 70(7 + (21)^{1/2})\nu k_6\}/(180\nu)).
\end{aligned} \tag{2}$$

If desired, a companion formula can be found by replacing $(21)^{1/2}$ throughout with $-(21)^{1/2}$. The parameter ν may have any value other than zero.

3. A Choice of Parameter. In some senses, a "best" formula is one for which each coefficient of k_i in expressions such as

$$f(x_n + h/2, y_n + \{(4\nu - 1)k_1 + k_2\}/(8\nu))$$

is positive or zero. If this is impossible, we may seek to minimize the sum of the absolute values of the coefficients. To establish a figure of merit, this sum should be divided by the weight 1/2 in $x_n + h/2$. In this connection see, for example, [5, p. 146]. The resulting expression for the above, assuming $\nu > 0$, is

$$1/(4\nu) + |1 - 1/(4\nu)| .$$

This is clearly nonincreasing, and is a minimum of 1 for $\nu \geqq 1/4$.

The other components of (2) behave in like manner except for that involving k_7, which is of the form $a/\nu + b$, where a and b are positive constants. Except for this component, the minimum is achieved for all if $\nu \geqq 4(55 + 9(21)^{1/2})/331 > 1$.

If the same tactics are applied to the formula resulting when $-(21)^{1/2}$ is used rather than $(21)^{1/2}$, it develops that all components are minimized if $\nu \geqq 1/4$ except that pertaining to k_5, which is of the form $a/\nu + b$, a and b positive.*

To determine whether to use the formula pertaining to $(21)^{1/2}$, as in (2), or that formed therefrom by replacing $(21)^{1/2}$ by $-(21)^{1/2}$, we need the actual minima. For $(21)^{1/2}$, in the order k_2, k_3, k_4, k_5, k_6, k_7, they are

$$1,\ 1,\ 1,\ 17/7,\ (232 + 33(21)^{1/2})/35,\ 4/(3\nu) + (526 + 259(21)^{1/2})/90 .$$

For $-(21)^{1/2}$, in the same order, they are

$$1,\ 1,\ 1,\ 4/(7\nu) + (55 + 3(21)^{1/2})/28,\ (41(21)^{1/2} - 13)/28,\ (130 + 63(21)^{1/2})/18 .$$

Since one is ideal, a comparison shows (the fundamental weights for y_{n+1} are also to be considered) that $-(21)^{1/2}$ is to be preferred, and that, if we desire $0 < \nu \leqq 1$, the value of ν should be one. The resulting k_i formulas are

* The author is indebted to the referee for pointing out that the sign of the surd might be used to advantage.

$$
\begin{aligned}
k_1 &= hf(x_n, y_n)\\
k_2 &= hf(x_n + h, y_n + k_1)\\
k_3 &= hf(x_n + h/2, y_n + \{3k_1 + k_2\}/8)\\
k_4 &= hf(x_n + 2h/3, y_n + \{8k_1 + 2k_2 + 8k_3\}/27)\\
k_5 &= hf(x_n + (7 - (21)^{1/2})h/14, y_n + \{3(3(21)^{1/2} - 7)k_1 - 8(7 - (21)^{1/2})k_2\\
&\qquad + 48(7 - (21)^{1/2})k_3 - 3(21 - (21)^{1/2})k_4\}/392)\\
k_6 &= hf(x_n + (7 + (21)^{1/2})h/14, y_n + \{-5(231 + 51(21)^{1/2})k_1\\
&\qquad - 40(7 + (21)^{1/2})k_2 - 320(21)^{1/2}k_3 + 3(21 + 121(21)^{1/2})k_4\\
&\qquad + 392(6 + (21)^{1/2})k_5\}/1960)\\
k_7 &= hf(x_n + h, y_n + \{15(22 + 7(21)^{1/2})k_1 + 120k_2\\
&\qquad + 40(7(21)^{1/2} - 5)k_3 - 63(3(21)^{1/2} - 2)k_4\\
&\qquad - 14(49 + 9(21)^{1/2})k_5 + 70(7 - (21)^{1/2})k_6\}/180).
\end{aligned}
\tag{3}
$$

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Department of Mathematics
Texas A&M University
College Station, Texas 77843

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