Runge-Kutta Methods with Constrained Minimum Error Bounds*

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Abstract. Optimum Runge-Kutta methods of orders $m = 2$, 3, and 4 are developed for the differential equation $y' = f(x, y)$ under Lotkin's conditions on the bounds for f and its partial derivatives, and with the constraint that the coefficient of $\partial^m f/\partial x^m$ in the leading error term be zero. The methods then attain higher order when it happens that f is independent of y.

1. Introduction. Anthony Ralston in [3] developed optimum Runge-Kutta methods of orders two, three, and four for a single first-order differential equation $y' = f(x, y)$. They are best in the sense that in each case the sum of the magnitudes of the coefficients in the leading truncation error term assumes a minimum under the following conditions: in the region of interest,

$$(1.1) \qquad |f(x, y)| < M \quad \text{and} \quad \left| \frac{\partial^{i+j} f}{\partial x^i \partial y^j} \right| < L^{i+j}/M^{j-1},$$

where M and L are constants and $i + j \leqq m$. These are the conditions used by Lotkin in [2]. Here, using Ralston's notation, the solution is to be advanced from x_0 to $x_1, x_2, \cdots$ by the mth-order Runge-Kutta approximation

$$(1.2) \qquad y_{n+1} = y_n + \sum_{i=1}^{m} w_i k_i ,$$

where $y_n = y(x_n)$, the w_i are constants,

$$(1.3) \qquad k_i = hf\left(x_n + \alpha_i h, y_n + \sum_{j=1}^{i-1} \beta_{ij} k_j\right),$$

and $h = x_{n+1} - x_n$. For each such approximation, it turns out that $\alpha_1 = 0$ and

$$(1.4) \qquad \alpha_i = \sum_{j=1}^{i-1} \beta_{ij} , \qquad i = 2, 3, \cdots , m.$$

The leading truncation error term, Eh^{m+1}, then satisfies

$$(1.5) \qquad | Eh^{m+1} | < cML^m h^{m+1};$$

Ralston minimized c as a function of the parameters to be determined. Other measures of the truncation error have been considered by Hull and Johnston [1].

Our purpose is to find optimum methods of orders $m = 2$, 3, and 4 which will attain higher order when it happens that f is independent of y. This requires that in each case the coefficient of $\partial^m f/\partial x^m$ (and, in fact, of $D^m f$) in the leading error term be zero; here D is defined as

$$(1.6) \qquad D = \partial/\partial x + f_n \, \partial/\partial y, \qquad f_n = f(x_n , y_n),$$

and

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$$D^s = \sum_{k=0}^{s} \binom{s}{k} f^k \partial^s / \partial x^{s-k} \partial y^k. \tag{1.7}$$

Furthermore, the vanishing of the term involving $D^m f$ implies that conditions (1.1) need only be satisfied for $i + j \leqq m - 1$.

2. Second-order Methods. The coefficient of h^3 in the error function is

$$E = [\tfrac{1}{6} - (\alpha_2^2 w_2/2)]D^2 f + [\tfrac{1}{6}] f_y Df. \tag{2.1}$$

Equating the coefficient of $D^2 f$ to zero yields

$$\alpha_2 = \tfrac{2}{3}, \qquad \beta_{21} = \tfrac{2}{3}, \qquad w_1 = \tfrac{1}{4}, \qquad w_2 = \tfrac{3}{4}, \tag{2.2}$$

so that the procedure becomes

$$y_{n+1} - y_n = (\tfrac{1}{4})hf(x_n, y_n) + (\tfrac{3}{4})hf(x_n + (\tfrac{2}{3})h, y_n + (\tfrac{2}{3})hf_n). \tag{2.3}$$

This is the same as Ralston's second-order method, and the truncation error is

$$| Eh^3 | < (\tfrac{1}{3}) ML^2 h^3. \tag{2.4}$$

In this instance, no minimization problem appears. For f independent of y the procedure becomes Radau quadrature of order 3.

3. Third-order Methods. Here the coefficient of h^4 in the error function is given by

$$E = a_1 D^3 f + a_2 f_y D^2 f + a_3 Df Df_y + a_4 f_y^2 Df, \tag{3.1}$$

where

$$\begin{aligned} a_1 &= \frac{1}{4!} - \frac{1}{3!}(\alpha_2^3 w_2 + \alpha_3^3 w_3), \\ a_2 &= \frac{1}{4!} - \frac{1}{2!}\alpha_2^2 \beta_{32} w_3, \\ a_3 &= \frac{3}{4!} - \alpha_2 \alpha_3 \beta_{32} w_3, \\ a_4 &= \frac{1}{4!}. \end{aligned} \tag{3.2}$$

But the vanishing of a_1 implies that

$$6\alpha_2\alpha_3 - 4(\alpha_2 + \alpha_3) + 3 = 0. \tag{3.3}$$

Along this hyperbola the error is bounded as follows:

$$| E | < [| a_2 | + | 2a_2 + a_3 | + | a_2 + a_3 | + 2| a_3 | + 2| a_4 |] ML^3, \tag{3.4}$$

with

$$\begin{aligned} a_2 &= \frac{1}{24} - \frac{\alpha_2}{12}, \\ a_3 &= \frac{1}{8} - \frac{\alpha_3}{6}, \\ a_4 &= \frac{1}{24}. \end{aligned} \tag{3.5}$$

If we now substitute (3.3) into (3.4) and minimize the right-hand side of (3.4) (as a function of α_2 or of α_3), we get $\alpha_2 = \frac{1}{3}$, $\alpha_3 = \frac{5}{6}$. With these parameter values the suggested procedure becomes

$$y_{n+1} - y_n = \tfrac{1}{10}k_1 + \tfrac{1}{2}k_2 + \tfrac{2}{5}k_3\,, \tag{3.6}$$

where

$$\begin{aligned} k_1 &= hf(x_n\,, y_n), \\ k_2 &= hf(x_n + \tfrac{1}{3}h,\ y_n + \tfrac{1}{3}k_1), \\ k_3 &= hf(x_n + \tfrac{5}{6}h,\ y_n - \tfrac{5}{12}k_1 + \tfrac{5}{4}k_2). \end{aligned} \tag{3.7}$$

The resulting bound on Eh^4 is

$$|\,Eh^4\,| < .1389ML^3h^4, \tag{3.8}$$

compared with $.1111ML^3h^4$, in Ralston's third-order procedure.

But if f is independent of y, then the procedure is fourth-order instead of third and the error bound is

$$|\,Eh^5\,| < 3.858 \times 10^{-5}ML^4h^5. \tag{3.9}$$

4. Fourth-order Methods. If we set to zero the coefficient

$$b_1 = \tfrac{1}{120} - \tfrac{1}{24}(\alpha_2^4 w_2 + \alpha_3^4 w_3 + w_4) \tag{4.1}$$

of D^4f in the leading error term, we again get an hyperbola in α_2 and α_3 :

$$10\alpha_2\alpha_3 - 5(\alpha_2 + \alpha_3) + 3 = 0. \tag{4.2}$$

Along this curve $b_3 = -4b_1$ vanishes also. The elements in

$$\begin{aligned} |\,E\,| < [8|\,b_2\,| + 8|\,b_4\,| + |\,b_5\,| + |\,2b_5 + b_7\,| + |\,b_5 + b_6 + b_7\,| \\ + |\,b_6\,| + |\,2b_6 + b_7\,| + |\,b_7\,| + 2|\,b_8\,|]ML^4 \end{aligned} \tag{4.3}$$

then become (see [1], p. 307)

$$\begin{aligned} &b_2 = \frac{5\alpha_3 - 3}{240}, \qquad b_4 = \frac{\alpha_3 - 1}{240(2\alpha_3 - 1)}, \qquad b_5 = -b_4 = \frac{1 - \alpha_3}{240(2\alpha_3 - 1)}, \\ &b_6 = \frac{(250\alpha_3^4 - 300\alpha_3^3 + 10\alpha_3^2 + 93\alpha_3 - 27)}{[(240)(10\alpha_3^2 - 12\alpha_3 + 3)]}, \\ &b_7 = \frac{2 - 5\alpha_3}{120}, \qquad b_8 = \frac{1}{120}. \end{aligned} \tag{4.4}$$

Minimizing the right-hand side of (4.3) along the hyperbola (4.2), we get

$$\alpha_2 = \frac{4 - (6)^{1/2}}{10} = .1550510257, \qquad \alpha_3 = \frac{4 + (6)^{1/2}}{10} = .6449489743, \tag{4.5a}$$

so that

$$
\begin{aligned}
&w_1 = 0, \qquad w_2 = \frac{16 - (6)^{1/2}}{36}, \qquad w_3 = \frac{16 + (6)^{1/2}}{36}, \qquad w_4 = \frac{1}{9}, \\
&\alpha_4 = 1, \qquad \beta_{21} = \frac{4 - (6)^{1/2}}{10}, \qquad \beta_{31} = -\left(\frac{11 + 4(6)^{1/2}}{25}\right), \\
&\beta_{32} = \frac{42 + 13(6)^{1/2}}{50}, \qquad \beta_{41} = \frac{1 + 5(6)^{1/2}}{4}, \\
&\beta_{42} = -\left(\frac{3 + 2(6)^{1/2}}{2}\right), \qquad \beta_{43} = \frac{9 - (6)^{1/2}}{4}.
\end{aligned} \tag{4.5b}
$$

This defines the following Runge-Kutta scheme:

$$y_{n+1} - y_n = .3764030627k_2 + .5124858262k_3 + .1111111111k_4, \tag{4.6}$$

with

$$
\begin{aligned}
k_1 &= hf(x_n, y_n), \\
k_2 &= hf(x_n + .1550510257h, y_n + .1550510257k_1), \\
k_3 &= hf(x_n + .6449489743h, y_n - .8319183588k_1 + 1.476867333k_2), \\
k_4 &= hf(x_n + h, y_n + 3.311862178k_1 - 3.949489743k_2 + 1.637627564k_3).
\end{aligned} \tag{4.7}
$$

The error bound is

$$|Eh^5| < \left(\frac{11 + 14(6)^{1/2}}{480}\right) ML^4h^5 = .0944ML^4h^5, \tag{4.8}$$

as compared with

$$|Eh^5| < .0546ML^4h^5 \tag{4.9}$$

for Ralston's fourth-order procedure.

In this case the method becomes fifth order when f is independent of y, with error bound

$$|Eh^6| < 1.389 \times 10^{-5}ML^5h^6. \tag{4.10}$$

5. An Additional Constraint. Now suppose we consider the second error term—that involving h^{m+2}. In this term, setting the coefficient of $D^{m+1}f$ to zero leads to

$$10\alpha_2\alpha_3 - 5(\alpha_2 + \alpha_3) + 3 = 0 \tag{5.1}$$

for third-order methods and to

$$2(\alpha_2^2\alpha_3 + \alpha_2\alpha_3^2) - (\alpha_2^2 - \alpha_2\alpha_3 + \alpha_3^2) - (\alpha_2 + \alpha_3) + 1 = 0 \tag{5.2}$$

for fourth-order methods. The intersection of (5.1) and (3.3) is the point

$$(\alpha_2, \alpha_3) = \left(\frac{6 - (6)^{1/2}}{10}, \frac{6 + (6)^{1/2}}{10}\right),$$

which determines the parameters

$$
(5.3) \quad \begin{aligned} w_1 &= \frac{1}{9}, \qquad w_2 = \frac{16 + (6)^{1/2}}{36}, \qquad w_3 = \frac{16 - (6)^{1/2}}{36}, \\ \beta_{21} &= \frac{6 - (6)^{1/2}}{10}, \qquad \beta_{31} = -\left(\frac{54 + 19(6)^{1/2}}{250}\right), \qquad \beta_{32} = \frac{102 + 22(6)^{1/2}}{125} \end{aligned}
$$

and thus defines the third-order procedure

$$
(5.4) \quad y_{n+1} - y_n = .1111111111k_1 + .5124858262k_2 + .3764030627k_3,
$$

where

$$
(5.5) \quad \begin{aligned} k_1 &= hf(x_n, y_n), \\ k_2 &= hf(x_n + .3550510257h, y_n + .3550510257k_1), \\ k_3 &= hf(x_n + .8449489743h, y_n - .4021612205k_1 + 1.247110195k_2), \end{aligned}
$$

with

$$
(5.6) \quad |Eh^4| < .1391ML^3h^4.
$$

For derivative functions f that are independent of y, this procedure becomes Radau quadrature of order five with leading error term

$$
(5.7) \quad |Eh^6| < 1.389 \times 10^{-5}ML^5h^6.
$$

Similarly, (5.2) and (4.2) intersect at

$$
(\alpha_2, \alpha_3) = \left(\frac{5 - (5)^{1/2}}{10}, \frac{5 + (5)^{1/2}}{10}\right)
$$

to yield

$$
(5.8) \quad \begin{aligned} & w_1 = \frac{1}{12}, \qquad w_2 = \frac{5}{12}, \qquad w_3 = \frac{5}{12}, \qquad w_4 = \frac{1}{12}, \\ & \alpha_4 = 1, \quad \beta_{21} = \frac{5 - (5)^{1/2}}{10}, \qquad \beta_{31} = -\left(\frac{5 + 3(5)^{1/2}}{20}\right), \quad \beta_{32} = \frac{3 + (5)^{1/2}}{4}, \\ & \beta_{41} = \frac{-1 + 5(5)^{1/2}}{4}, \qquad \beta_{42} = -\left(\frac{5 + 3(5)^{1/2}}{4}\right), \qquad \beta_{43} = \frac{5 - (5)^{1/2}}{2}. \end{aligned}
$$

This is the fourth-order system

$$
(5.9) \quad \begin{aligned} y_{n+1} - y_n = {} & .08333333333k_1 + .4166666667k_2 + .4166666667k_3 \\ & + .08333333333k_4, \end{aligned}
$$

where

$$
(5.10) \quad \begin{aligned} k_1 &= hf(x_n, y_n), \\ k_2 &= hf(x_n + .2763932023h, y_n + .2763932023k_1), \\ k_3 &= hf(x_n + .7236067977h, y_n - .5854101966k_1 + 1.309016994k_2), \\ k_4 &= hf(x_n + h, y_n + 2.545084972k_1 - 2.927050983k_2 + 1.381966011k_3), \end{aligned}
$$

with

$$
(5.11) \quad |Eh^5| < .1218ML^4h^5.
$$

For f independent of y, (5.9, 10) is Lobatto's sixth-order quadrature formula, with truncation error

$$|Eh^7| < 6.614 \times 10^{-7} ML^6 h^7. \tag{5.12}$$

The restriction that $\alpha_4 = 1$, however, precludes having a fourth-order integration scheme corresponding to Radau quadrature, which in this case is of order seven.

6. Examples. Both of Ralston's examples and several others have been programmed for a CONTROL DATA 3600 computer, using all of the proposed methods. Results were as good as those for the Ralston schemes. Furthermore, the suggested procedures (3.6, 7), (4.6, 7), (5.4, 5), and (5.9, 10) did indeed produce results of the predicted order of accuracy when the example

$$y' = y, \qquad y(0) = 1, \qquad \text{solution } y(x) = e^x \tag{6.1}$$

was redone with $y' = e^x$. That is, the integration procedures reduce to high-order quadrature formulas and thus could be used to do double duty in a subroutine library.

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