MATHEMATICS OF COMPUTATION, VOLUME 25, NUMBER 115, JULY, 1971

Some Relations Between the Values of a Function and its First Derivative at n Abscissa Points

By Robert E. Huddleston

Abstract. For a polynomial, P, of degree $2n - 2$, there exists a relation between the values of P and the values of its first derivative, P', at the n abscissa points $x_1, \cdots, x_n$,

$$\sum_{i=1}^{n} [a_i P(x_i) + b_i P'(x_i)] = 0.$$

Replacing P by a differentiable function y yields

$$\sum_{i=1}^{n} [a_i y(x_i) + b_i y'(x_i)] = E(y, x).$$

These relations are obtained and the error function $E(y, x)$ is given explicitly.

1. Introduction. For a polynomial, P_{2n-2}, of degree $2n - 2$, there exists a relation between the values of P_{2n-2} and its first derivative at the n distinct abscissas $x_1, \cdots, x_n$. If $n = 2$ and $x_2 - x_1 = h$, the relation is

$$2P_2(x_1) + hP_2'(x_1) = 2P_2(x_2) - hP_2'(x_2).$$

If we impose the condition that $x_j = x_1 + (j - 1)h$, $j = 1, 2, \cdots, n$ (fixed step-size case), then at least for low-order n, there is a reasonably straightforward method for determining such relations [1, p. 247]. If we are given a function y which is differentiable, how much error do we incur by using the polynomial relation for y? For $n = 2$, we are asking what the term $E(x, y)$ is in the relation

$$2y(x_1) + hy'(x_1) = 2y(x_2) - hy'(x_2) + E(x, y).$$

For the fixed step-size case and for $n \leqq 4$, these relations are in the literature [1, p. 247]. However, for the case in which the x_i are not evenly spaced, no such results are available. It is the purpose of this paper to derive such relations along with the corresponding error relations.

2. Method. Let $y_j \equiv y(x_j)$ and $y_j' \equiv y'(x_j)$, $j = 1, \cdots, n$. We shall use a method which in essence is the derivation of Hermite interpolation, given the data $(x_1, y_1, y_1'), \cdots, (x_{n-1}, y_{n-1}, y_{n-1}'), (x_n, y_n')$. The lack of data for y_n causes most of the difficulties. However, if one is familiar with the derivation of Hermite interpolation [3, p. 192], the derivation of the following relations will be recognized as an exercise in drudgery. The determination of the relation for $E(x, y)$ is not so straightforward. Hence, we shall first determine the polynomial P_{2n-2} such that $P_{2n-2}(x_i) = y_i$, $i = 1,$

Received June 25, 1970.

AMS 1970 *subject classifications.* Primary 65L05; Secondary 26A75.

Key words and phrases. Ordinary differential equations, Runge-Kutta, error estimation for Runge-Kutta, one-step methods for ordinary differential equations, polynomials.

$\cdots, n-1$, and $P'_{2n-2}(x_i) = y'_i$, $i = 1, \cdots, n$. Then, we will evaluate the polynomial at x_n and find $E(x_n, y)$ such that

$$y(x_n) = P_{2n-2}(x_n) + E(x_n, y).$$

3. Derivation of P_{2n-2}. Following the idea of Hermite interpolation, we search for P_{2n-2} of the form

$$P_{2n-2}(x) = \sum_{i=1}^{n-1} \alpha_i(x) y_i + \sum_{i=1}^{n} \beta_i(x) y'_i, \tag{3.1}$$

where

$$\alpha_i(x_j) = \delta_{ij}, \quad j = 1, \cdots, n-1, \qquad \beta_i(x_j) = 0, \quad j = 1, \cdots, n-1,$$
and
$$\alpha'_i(x_j) = 0, \quad j = 1, \cdots, n, \qquad \beta'_i(x_j) = \delta_{ij}, \quad j = 1, \cdots, n.$$

Let

$$l_i(x) = \frac{1}{A_i} \prod_{j=1; j\neq i}^{n-1} (x - x_j)$$

where

$$A_i = \prod_{j=1; j\neq i}^{n-1} (x_i - x_j).$$

The α_i can then be represented by

$$\alpha_i(x) = A_i^2 l_i^2(x)[\gamma_i x^2 + \delta_i x + \eta_i],$$

where the γ_i, δ_i, and η_i are to be determined by the conditions $\alpha_i(x_i) = 1$, $\alpha'_i(x_i) = \alpha'_i(x_n) = 0$. After much algebraic manipulation we arrive at

$$\gamma_i = \frac{1}{A_i^2(x_n - x_i)} \left[l'_i(x_i) + \frac{l'_i(x_n)[(x_n - x_i) l'_i(x_i) - 1]}{l_i(x_n) + (x_n - x_i) l'_i(x_n)} \right],$$

$$\delta_i = -2A_i^{-2} l'_i(x_i) - 2\gamma_i x_i,$$

$$\eta_i = A_i^{-2} + 2A_i^{-2} x_i l'_i(x_i) + x_i^2 \gamma_i.$$

Since we are interested in evaluating $P_{2n-2}(x)$ at x_n, we find

$$\alpha_i(x_n) = -l_i^2(x_n) \left[\sum_{j=1}^{n-1} \frac{1}{x_n - x_j} \right]^{-1} \left[\sum_{j=1; j\neq i}^{n} \frac{1}{x_i - x_j} \right]. \tag{3.2}$$

In like manner the β_i, for $i = 1, \cdots, n-1$, may be represented by

$$\beta_i(x) = A_i^2 l_i^2(x)[a_i x^2 + b_i x + c_i]$$

where the a_i, b_i, and c_i are to be determined by $\beta_i(x_i) = \beta'_i(x_n) = 0$ and $\beta'_i(x_i) = 1$. This yields

$$a_i = -\frac{1}{2A_i^2} \left[\frac{1}{x_n - x_i} + \frac{l'_i(x_n)}{l_i(x\ ) + (x_n - x_i) l'_i(x_n)} \right],$$

and

$$b_i = A_i^{-2} - 2a_i x_i,$$

$$c_i = x_i[a_i x_i - A_i^{-2}].$$

The term $\beta_n(x)$ is determined separately and yields

$$\beta_n(x) = \frac{l_n^2(x)}{2l_n'(x_n)}.$$

Combining these relations for the β_i and evaluating at x_n, we have

$$\beta_i(x_n) = \tfrac{1}{2} l_i^2(x_n)\left[\sum_{j=1}^{n-1} \frac{1}{x_n - x_j}\right]^{-1}, \qquad j = 1, \cdots, n. \tag{3.3}$$

From (3.1), (3.2), and (3.3), we have

$$\begin{aligned} &P_{2n-2}(x_n) \\ &= \left(\sum_{j=1}^{n-1} \frac{1}{x_n - x_j}\right)^{-1}\left\{-\sum_{i=1}^{n-1}\left[l_i^2(x_n)\left(\sum_{j=1;j\neq i}^{n} \frac{1}{x_i - x_j}\right)y_i\right] + \frac{1}{2}\sum_{i=1}^{n} l_i^2(x_n)y_i'\right\}. \end{aligned} \tag{3.4}$$

4. Determination of the Error. We now wish to determine $E(y, x_n)$ in the relation

$$y(x_n) = P_{2n-2}(x_n) + E(y, x_n).$$

Let

$$\phi(x) = 2(x_n - x)l_n^2(x)l_n'(x_n) + l_n^2(x). \tag{4.1}$$

Then

$$\phi(x_j) = \delta_{nj}, \qquad j = 1, \cdots, n,$$

$$\phi'(x_j) = 0, \qquad j = 1, \cdots, n.$$

Let F be defined by

$$F(x) = y(x) - P_{2n-2}(x) - \phi(x)[y(x_n) - P_{2n-2}(x_n)]. \tag{4.2}$$

Then F has the properties

$$\begin{aligned} F(x_j) &= 0, \qquad j = 1, \cdots, n, \quad \text{and} \\ F'(x_j) &= 0, \qquad j = 1, \cdots, n. \end{aligned} \tag{4.3}$$

Hence, F has at least $2n$ zeroes (n double zeroes) in the smallest interval J containing $x_1, \cdots, x_n$. [Note that $l_n'(x_n)$ is nonzero provided that x_n lies outside the smallest interval, I, containing $x_1, \cdots, x_{n-1}$.] Applying Rolle's theorem $(2n - 1)$ times, we may state that $F^{(2n-1)}$ has at least one zero in J. Let ζ be such a zero. From (4.2),

$$F^{(2n-1)}(x) = y^{(2n-1)}(x) - P_{2n-2}^{(2n-1)}(x) - \phi^{(2n-1)}(x)[y(x_n) - P_{2n-2}(x_n)].$$

But $P_{2n-2}^{(2n-1)}(x) \equiv 0$ since the degree of $P_{2n-2}(x) = 2n - 2$. If one notes that $\phi(x)$ is a polynomial of degree $2n - 1$ with leading coefficient $-2A_n^{-2}l_n'(x_n)$, then it is clear that

$$\phi^{(2n-1)}(x) = -2(2n - 1)!\ A_n^{-2}l_n'(x_n).$$

Hence,

$$0 = F^{(2n-1)}(\zeta) = y^{(2n-1)}(\zeta) + 2(2n-1)!\ A_n^{-2} l_n'(x_n)[y(x_n) - P_{2n-2}(x_n)].$$

Thus, we have established the following:

THEOREM. *If* $y \in C^{(2n-1)}[J]$, *then*

$$y(x_n) = P_{2n-2}(x_n) - \frac{A_n^2 y^{(2n-1)}(\zeta)}{2(2n-1)!\ l_n'(x_n)}, \tag{4.4}$$

where $\zeta \in J$ *and* $x_n \notin I$.

5. Relations Between $y(x_j)$ and $y'(x_j)$. From (3.4) and (4.4) and use of the identity

$$l_i'(x) = l_i(x) \sum_{j=1;j\neq i}^{n-1} \frac{1}{x_i - x_j},$$

we arrive at the desired relation between $y(x_j)$ and $y'(x_j)$, $j = 1, \cdots, n$:

$$\sum_{i=1}^{n} \left\{ \prod_{j=1;j\neq i}^{n-1} \left(\frac{x_n - x_j}{x_i - x_j} \right)^2 \left[y_i' - \left(\sum_{j=1;j\neq i}^{n} \frac{2}{x_i - x_j} \right) y_i \right] \right\} = -E(x_n, y) \tag{5.1}$$

where

$$E(x_n, y) = -\frac{\prod_{j=1}^{n-1} (x_n - x_j)^2 y^{(2n-1)}(\zeta)}{2(2n-1)!\ \sum_{j=1}^{n-1} \left(\frac{1}{x_n - x_j} \right)}. \tag{5.2}$$

For the special case of even step-size ($x_j = x_1 + (j-1)h$, $j = 1, \cdots, n$), the above relations reduce to

$$\sum_{i=1}^{n} \left\{ \binom{n-1}{i-1} \left[hy_i' - \left(\sum_{j=1;j\neq i}^{n} \frac{2}{i-j} \right) y_i \right] \right\} = -E(x_n, y), \tag{5.3}$$

where

$$E(x_n, y) = -\frac{[(n-1)!]^2}{2(2n-1)!} h^{2n-1} y^{(2n-1)}(\zeta). \tag{5.4}$$

6. An Alternate Approach. If we had given the data $(x_1, y_1, y_1'), \cdots, (x_{n-1}, y_{n-1}, y_{n-1}'), (x_n, y_n)$ and determined the polynomial

$$Q_{2n-2}(x) = \sum_{i=1}^{n} q_i(x) y_i + \sum_{i=1}^{n-1} r_i(x) y_i' \tag{6.1}$$

such that

$$Q_{2n-2}(x_i) = y_i, \qquad i = 1, \cdots, n,$$

$$Q_{2n-2}'(x_i) = y_i', \qquad i = 1, \cdots, n-1,$$

we would have had a much easier task in deriving expressions for the q_i and r_i. We could have then determined $e(x, y)$ such that

$$y(x) = Q_{2n-2}(x) + e(x, y). \tag{6.2}$$

Having done this, we could differentiate (6.1), evaluate it at x_n, and have the desired relationship between $y(x_j)$ and $y'(x_j)$ for $j = 1, \cdots, n$. However, the proof that $e(x, y)$ can be differentiated as a function of x and the resulting differentiation represent a considerable task. From (6.1) and (6.2), we may write

$$(6.3)\qquad y_n = \sum_{i=1}^{n-1}\left(-\frac{q_i'(x_n)}{q_n'(x_n)}y_i\right) + \sum_{i=1}^{n-1}\left(-\frac{r_i'(x_n)}{q_n'(x_n)}y_i'\right) + \frac{y'(x_n)}{q_n'(x_n)} - \frac{e'(x_n, y)}{q_n'(x_n)}$$

which we may compare with

$$(6.4)\qquad y_n = \sum_{i=1}^{n-1} \alpha_i(x_n)y_i + \sum_{i=1}^{n} \beta_i(x_n)y_i' + E(x_n, y).$$

Choosing y to be an arbitrary polynomial of degree exactly $2n - 2$, we note that the error terms are zero. Noting also that (1) the coefficients α_i, β_i, q_i, and r_i are independent of y, and (2) that the relation between the values of a polynomial of degree $2n - 2$ and its derivatives at n distinct abscissa points is unique, we arrive at the conclusion that

$$\alpha_i(x_n) = -\frac{q_i'(x_n)}{q_n'(x_n)} \quad\text{and}\quad \beta_i(x_n) = -\frac{r_i'(x_n)}{q_n'(x_n)},$$

$$\text{for}\quad i = 1, \cdots, n-1 \quad\text{and}\quad \beta_n(x_n) = \frac{1}{q_n'(x_n)}.$$

But then from (6.3) and (6.4), we conclude that

$$e_n'(x_n, y) = -q_n'(x_n)E(x_n, y).$$

7. Applications to Differential Equations. In order to approximate the solution of the initial-value problem

$$(7.1)\qquad y'(x) = f(x, y(x)), \qquad y(a) = A,$$

one often uses a one-step scheme of the form

$$(7.2)\qquad y_{n+1} = y_n + h\Phi(x_n, y_n, h_n), \qquad y_0 = A,$$

where $h_n = x_{n+1} - x_n$. The local truncation error, τ_n, in proceeding from x_n to x_{n+1}, is defined by

$$(7.3)\qquad \tau_n = Z(x_{n+1}) - y_{n+1}$$

where $Z(x)$ is given by

$$(7.4)\qquad Z'(x) = f(x, Z(x)), \qquad Z(x_n) = y_n.$$

Using the relationship (5.3) for Z with $n = 2$, we have

$$2Z(x_n) + hZ'(x_n) = 2Z(x_{n+1}) - hZ'(x_{n+1}) + O(h^3),$$

which, from (7.3) and (7.4), yields

$$(7.5)\qquad 2y_n + hf(x_n, y_n) = 2[\tau_n + y_{n+1}] - hf(x_{n+1}, \tau_n + y_{n+1}) + O(h^3).$$

Using a Taylor series expansion, we have

$$f(x_{n+1}, \tau_n + y_{n+1}) = f(x_{n+1}, y_{n+1}) + f_y(x_{n+1}, y_{n+1})\tau_n + O(\tau_n^2).$$

Substituting this in (7.5), we have

$$\tau_n = [y_n - y_{n+1}] + \tfrac{1}{2}h[f(x_n, y_n) + f(x_{n+1}, y_{n+1})] + hf_y(x_{n+1}, y_{n+1})\tau_n + O(h\tau_n^2). \tag{7.6}$$

If this estimate is used with a one-step method having local truncation error of order h^2 (for example, Euler's method), then the last two terms of (7.6) are of the order h^3 and h^5 and, hence, are negligible with respect to the local truncation error. Thus, we have the estimate

$$\tau_n = [y_n - y_{n+1}] + \tfrac{1}{2}h[f(x_n, y_n) + f(x_{n+1}, y_{n+1})]. \tag{7.7}$$

Such estimates are derivable for one-step methods of higher order through the use of relation (5.1). The extensions are not straightforward and constitute the subject of [2]. It is important to note that the quantities needed for the estimate (7.7) are those normally calculated in a one-step procedure and thus require no additional function evaluations. This property is characteristic of estimates derivable from (5.1) (see [2]) and thus results in error estimates which are very inexpensive with respect to computer time. In particular, the estimates can replace the time consuming process, so often used with Runge-Kutta, of carrying two simultaneous calculations with step-sizes h and $2h$ and comparing the answers for step-size control.

Sandia Laboratories
Numerical Applications Division 8321
Livermore, California 94550

1. F. Ceschino & J. Kuntzmann, *Numerical Solution of Initial Value Problems*, Prentice-Hall, Englewood Cliffs, N. J., 1966. MR **33** #3465.
2. R. E. Huddleston, *Variable-Step Truncation Error Estimates for Runge-Kutta Methods of Order* 4 *or Less*, Report #DC-70-261, Sandia Laboratories, Livermore, California.
3. E. Isaacson & H. B. Keller, *Analysis of Numerical Methods*, Wiley, New York, 1966. MR **34** #924.