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

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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 $x_1, \dots, x_n$,

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

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 $x_1, \dots, x_n$. 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 $x_j = x_1 + (j - 1)h$, $j = 1, 2, \dots, n$ (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 $n \leq 4$, 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 $y_i \equiv y(x_i)$ and $y'_i \equiv y'(x_i)$, $j = 1, \dots, n$. We shall use a method which in essence is the derivation of Hermite interpolation, given the data $(x_1, y_1, y'_1), \dots, (x_{n-1}, y_{n-1}, y'_{n-1}), (x_n, y'_n)$. 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 $P_{2n-2}(x_i) = y_i$, $i = 1,$

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$\dots, n-1$, and $P'_{2n-2}(x_i) = y'_i$, $i = 1, \dots, n$. 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

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

where

$$\begin{aligned} \alpha_i(x_j) &= \delta_{ij}, & j &= 1, \dots, n-1, & \text{and} & \beta_i(x_j) &= 0, & j &= 1, \dots, n-1, \\ \alpha'_i(x_j) &= 0, & j &= 1, \dots, n, & \beta'_i(x_j) &= \delta_{ij}, & j &= 1, \dots, n. \end{aligned}$$

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

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

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

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

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

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

In like manner the β_i , for $i = 1, \dots, n-1$, 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

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

and

$$\begin{aligned}b_i &= A_i^{-2} - 2a_i x_i, \\c_i &= x_i[a_i x_i - A_i^{-2}].\end{aligned}$$

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

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

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

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

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

$$(4.1) \quad \phi(x) = 2(x_n - x)l_n^2(x)l'_n(x_n) + l_n^2(x).$$

Then

$$\begin{aligned}\phi(x_j) &= \delta_{nj}, & j &= 1, \dots, n, \\ \phi'(x_j) &= 0, & j &= 1, \dots, n.\end{aligned}$$

Let F be defined by

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

Then F has the properties

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

Hence, F has at least $2n$ zeroes (n double zeroes) in the smallest interval J containing $x_1, \dots, x_n$. [Note that $l'_n(x_n)$ is nonzero provided that x_n lies outside the smallest interval, I , containing $x_1, \dots, x_{n-1}$.] 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,

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

Thus, we have established the following:

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

$$(4.4) \quad y(x_n) = P_{2n-2}(x_n) - \frac{A_n^2 y^{(2n-1)}(\xi)}{2(2n-1)! l'_n(x_n)},$$

where $\xi \in J$ and $x_n \notin I$.

5. Relations Between $y(x_i)$ and $y'(x_i)$. 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 $y(x_i)$ and $y'(x_i)$, $j = 1, \dots, n$:

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

where

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

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

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

where

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

6. An Alternate Approach. If we had given the data $(x_1, y_1, y'_1), \dots, (x_{n-1}, y_{n-1}, y'_{n-1}), (x_n, y_n)$ and determined the polynomial

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

such that

$$\begin{aligned} Q_{2n-2}(x_i) &= y_i, & i &= 1, \dots, n, \\ Q'_{2n-2}(x_i) &= y'_i, & i &= 1, \dots, n-1, \end{aligned}$$

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

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

Having done this, we could differentiate (6.1), evaluate it at x_n , and have the desired relationship between $y(x_i)$ and $y'(x_i)$ for $j = 1, \dots, n$. 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

$$(6.3) \quad y_n = \sum_{i=1}^{n-1} \left(-\frac{q'_i(x_n)}{q'_n(x_n)} y_i \right) + \sum_{i=1}^{n-1} \left(-\frac{r'_i(x_n)}{q'_n(x_n)} y'_i \right) + \frac{y'(x_n)}{q'_n(x_n)} - \frac{e'(x_n, y)}{q'_n(x_n)}$$

which we may compare with

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

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

$$\alpha_i(x_n) = -\frac{q'_i(x_n)}{q'_n(x_n)} \quad \text{and} \quad \beta_i(x_n) = -\frac{r'_i(x_n)}{q'_n(x_n)},$$

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

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

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

one often uses a one-step scheme of the form

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

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

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

where $Z(x)$ is given by

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

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

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

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

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

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

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

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.

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