High Accuracy Quadrature Formulas from Divided Differences with Repeated Arguments

In the numerical solution of differential equations, one uses quadrature formulas to relate the unknown functions to their derivatives. While the functions enter only at the beginning and end of the range of integration, all intermediate values of the derivatives may enter. For checking purposes at least, it would be advantageous to increase the accuracy of the quadrature formulas by permitting weights to be assigned to intermediate values of the functions, as well as their derivatives. An interesting method of obtaining such formulas is given below.

Given a function $f(x)$ and $n + 1$ distinct values of the argument $x_0, x_1, \cdots, x_n$, the nth order divided difference of $f(x)$ with respect to these values of x may be defined as

$$(1) \qquad f(x_0, x_1, \cdots, x_n) = \sum_{p=0}^{n} \frac{f(x_p)}{\Pi_p},$$

where

$$(2) \qquad \Pi_p = \prod_{\substack{i=0 \\ i \neq p}}^{n} (x_p - x_i);$$

for example,

$$(3) \quad f(x_0 x_1, x_2) = \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} + \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)}.$$

An upper limit can be obtained for the value of a divided difference by means of the following theorem, see [1]. If $f(x)$ and its first $n - 1$ derivatives are finite and continuous and the nth derivative $f^{(n)}(x)$ exists, then

$$(4) \qquad f(x_0, x_1, \cdots, x_n) = \frac{f^{(n)}(\xi)}{n!},$$

where ξ lies in the range between the smallest and largest of the arguments x_0 to x_n.

For a divided difference involving a repeated argument one takes the limit as two initially distinct arguments approach one another; thus

$$(5) \quad f(x_0, x_0) = \lim_{x_0' \to x_0} f(x_0', x_0) = \lim_{x_0' \to x_0} \left[\frac{f(x_0')}{x_0' - x_0} + \frac{f(x_0)}{x_0 - x_0'} \right] = \frac{d}{dx_0} f(x_0).$$

In general, as shown in [2],

$$(6) \quad f(\overbrace{x_0, \cdots, x_0}^{k_0 + 1}, \overbrace{x_1, \cdots, x_1}^{k_1 + 1}, \overbrace{x_n, \cdots, x_n}^{k_n + 1})$$

$$= \frac{1}{k_0! k_1! \cdots k_n!} \frac{\partial k_0 + k_1 + \cdots + k_n}{\partial x_0^{k_0} \partial x_1^{k_1} \cdots \partial x_n^{k_n}} f(x_0, x_1, \cdots, x_n)$$

and, for the special case $k_i = k$, for all i,

$$F_k \equiv f(\overbrace{x_0, \cdots, x_0}^{k+1}, \overbrace{x_1, \cdots, x_1}^{k+1}, \cdots, \overbrace{x_n, \cdots, x_n}^{k+1}) = \frac{1}{(k!)^{n+1}} \left[\prod_{i=0}^{n} \frac{\partial^k}{\partial x_i^k} \right] \sum_{p=0}^{n} \frac{f(x_p)}{\Pi_p}, \tag{7}$$

where Π_p is given by (2).

From (7)

$$F_k = \frac{1}{(k!)^{n+1}} \sum_{p=0}^{n} \left[\prod_{i=0}^{n} \frac{\partial^k}{\partial x_i^k} \right] \frac{f(x_p)}{\Pi_p} = \frac{1}{(k!)^{n+1}} \sum_{p=0}^{n} \frac{\partial^k}{\partial x_p^k} \left\{ f(x_p) \left[\prod_{\substack{i=0 \\ i \neq p}}^{n} \frac{\partial^k}{\partial x_i^k} \right] \frac{1}{\Pi_p} \right\}, \tag{8}$$

and since in (8)

$$\frac{\partial^k}{\partial x_i^k} \frac{1}{\Pi_p} = \frac{k!}{(x_p - x_i)^k} \frac{1}{\Pi_p}, \quad \text{for} \quad i \neq p, \tag{9}$$

one has

$$F_k \equiv f(\overbrace{x_0, \cdots, x_0}^{k+1}, \cdots, \overbrace{x_n, \cdots, x_n}^{k+1}) = \frac{1}{k!} \sum_{p=0}^{n} \frac{\partial^k}{\partial x_p^k} \frac{f(x_p)}{\Pi_p^{k+1}}. \tag{10}$$

Therefore by Leibnitz's Theorem

$$f(\overbrace{x_0, \cdots, x_0}^{k+1}, \cdots, \overbrace{x_n, \cdots, x_n}^{k+1}) = \sum_{p=0}^{n} \sum_{s=0}^{k} N_p^s f^{(s)}(x_p), \tag{11}$$

where $f^{(s)}(x_p)$ represents the sth derivative of $f(x_p)$ and

$$N_p^s \equiv \frac{1}{s!(k-s)!} \frac{\partial^{k-s}}{\partial x_p^{k-s}} \frac{1}{\Pi_p^{k+1}}. \tag{12}$$

Special Case $k = 1$

From (12)

$$N_p^0 = \frac{\partial}{\partial x_p} \Pi_p^{-2} = -2\Pi_p' \Pi_p^{-3} \tag{13}$$

$$N_p^1 = \Pi_p^{-2}$$

where

$$\Pi_p' \equiv \frac{\partial \Pi_p}{\partial x_p} = \Pi_p \sum_{\substack{j=0 \\ j \neq p}}^{n} \frac{1}{x_p - x_j}. \tag{14}$$

For equally spaced arguments $x_i = x_0 + ih$, where $i = 0, 1, \cdots, n$, one has from (2)

$$\Pi_p = (-1)^{n-p} p!(n-p)!h^n. \tag{15}$$

Likewise, from (14)

$$\Pi_p' = (-1)^{n-p} p!(n-p)![S_p - S_{n-p}]h^{n-1}, \tag{16}$$

where $S_0 = 0$ and

$$S_r = \sum_{i=1}^{r} \frac{1}{i}, \quad \text{for} \quad r \neq 0; \tag{17}$$

therefore, from (13)

$$\begin{aligned} N_p^0 &= \frac{-2[S_p - S_{n-p}]}{h^{2n+1}[p!(n-p)!]^2} \\ N_p^1 &= \frac{1}{h^{2n}[p!(n-p)!]^2}. \end{aligned} \tag{18}$$

Multiplying (11) through by $(n!)^2 h^{2n+1}$ and making use of (4), one has

$$\sum_{p=0}^{n} A_{np} f(x_p) = h \sum_{p=0}^{n} B_{np} f^{(1)}(x_p) - \frac{h^{2n+1}}{D_n} f^{(2n+1)}(\xi), \tag{19}$$

where $x_0 < \xi < x_n$, and one sets

$$A_{np} = 2[S_p - S_{n-p}][C_p^n]^2 \tag{20}$$

$$B_{np} = [C_p^n]^2 \tag{21}$$

and

$$D_n = \frac{(2n+1)!}{(n!)^2}. \tag{22}$$

In the above equations

$$C_p^n = \frac{n!}{p!(n-p)!} \tag{23}$$

are the binomial coefficients.

The first two quadrature formulas corresponding to $n = 1$ and $n = 2$ are the trapezoidal rule and Simpson's rule, respectively, applied to the derivative of $f(x)$. The formulas for higher value of n have the usually undesirable feature of involving the value of the integrated function $f(x)$ at intermediate values of x between x_0 and x_n. They should, however, due to their very small remainder terms, prove useful in checking the accuracy of integration in the numerical solution of differential equations. Moreover, these quadrature formulas should be advantageous in the solution of two-point boundary value problems, since these must be solved by a relaxation or by an iteration method.

K. S. Kunz

Schlumberger Well Surveying Corp.
Ridgefield, Connecticut

1. L. M. Milne-Thomson, *The Calculus of Finite Differences*, Macmillan & Company, London, 1933, p. 5–6.
2. *Ibid.*, p. 14.

Tables of the coefficients in (19) are given below:

TABLE 1

Coefficients A_{np}

$n \backslash p$	0	1	2	3	4	5	6
1	-2	2					
2	-3	0	3				
3	$-\frac{11}{3}$	-9	9	$\frac{11}{3}$			
4	$-\frac{25}{6}$	$-\frac{80}{3}$	0	$\frac{80}{3}$	$\frac{25}{6}$		
5	$-\frac{137}{30}$	$-\frac{325}{6}$	$-\frac{200}{3}$	$\frac{200}{3}$	$\frac{325}{6}$	$\frac{137}{30}$	
6	$-\frac{49}{10}$	$-\frac{462}{5}$	$-\frac{525}{2}$	0	$\frac{525}{2}$	$\frac{462}{5}$	$\frac{49}{10}$

TABLE 2

Coefficients B_{np}

$n \backslash p$	0	1	2	3	4	7	6	D_n
1	1	1						6
2	1	4	1					30
3	1	9	9	1				140
4	1	16	36	16	1			630
5	1	25	100	100	25	1		2772
6	1	36	225	400	225	36	1	12012