Integration Formulae Involving Derivatives

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Abstract. A method, developed by Hammer and Wicke, for deriving high precision integration formulae involving derivatives is modified. It is shown how such formulae may be simply derived in terms of well-known polynomials. ■

1. Introduction. The construction of high precision integration formulae which make use of the derivatives of the integrand has been discussed by Stroud and Stancu [1] and by Hammer and Wicke [2]. Stroud and Stancu [1] considered formulae of the form

$$\int_a^b w(x)f(x)dx = \sum_{j=1}^{n} \sum_{i=0}^{k_j-1} H_j^{(i)} f^{(i)}(x_j) \tag{1}$$

and have calculated a few results for the special case, $k_j = k$, for all j, with $n = 1(1)7$, $k = 3$ and 5 and $w(x) = 1$, e^{-x^2} and e^{-x}. The formulae have degree $n(k+1) - 1$, use nk functional evaluations and are obtained by solving sets of nonlinear equations.

Hammer and Wicke [2] considered formulae of the form

$$\int_{-1}^{1} f(x)dx = 2 \sum_{i=0}^{[(k-1)/2]} f^{(2i)}(0)/(2i+1)! + \sum_{j=1}^{m} a_j[f^{(k)}(x_j) - f^{(k)}(-x_j)] \tag{2}$$

where $[x]$ denotes the largest integer $\leqq x$. These formulae have degree $4m + k$ when k is odd and $4m + k - 1$ when k is even and use $2m + 1 + [(k-1)/2]$ function values. The m abscissae x_j are the zeros of a numerically determined orthogonal polynomial. Struble [3] has calculated formulae for the cases $k = 1$ and 2 and $m = 1(1)10$. He notes that some numerical difficulties occur for large values of m. The formulae of Stroud and Stancu [1] use about twice as many function values as the Hammer and Wicke [2] formulae for the same integrating degree and are much more difficult to obtain.

This paper is concerned with formulae of the Hammer and Wicke type. It is shown that with a slight decrease in integrating power the derivation of the formula can be simplified and some results are presented.

2. Theory. The formulae of Hammer and Wicke [2] are based on the well-known result that

$$\int_0^1 \left(\int_0^x\right)^n g(x)\,(dx)^{n+1} = \frac{1}{n!}\int_0^1 (1-x)^n g(x)dx \tag{3}$$

where $(\int_0^x)^n g(x)(dx)^n$ denotes repeated integration over $[0, x]$.

It is equally true that

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$$\int_{-1}^{1} \left(\int_{-1}^{x} \right)^{n} g(x)\,(dx)^{n+1} = \frac{1}{n!} \int_{-1}^{1} (1 - x)^{n} g(x) dx \,. \tag{4}$$

It is straightforward to show by repeated integration of $f^{(k)}(x)$ that,

$$\int_{-1}^{1} \left(\int_{-1}^{x} \right)^{k} f^{(k)}(x)\,(dx)^{k+1} = \int_{-1}^{1} f(x) dx - \sum_{i=0}^{k-1} \frac{2^{i+1}}{(i+1)!} f^{(i)}(-1) \,. \tag{5}$$

Thus using (4) gives,

$$\int_{-1}^{1} f(x) dx = \frac{1}{k!} \int_{-1}^{1} (1 - x)^{k} f^{(k)}(x) dx + \sum_{i=0}^{k-1} \frac{2^{i+1}}{(i+1)!} f^{(i)}(-1) \tag{6}$$

$$= \frac{1}{k!} \sum_{j=1}^{m} H_j f^{(k)}(x_j) + \sum_{i=0}^{k-1} \frac{2^{i+1}}{(i+1)!} f^{(i)}(-1) + \frac{2^{k+2m+1}}{(k+2m+1)(2m)!k!} \left[\frac{m!(k+m)!}{(k+2m)!} \right]^{2} f^{(2m+k)}(\eta) \,. \tag{7}$$

In the remainder term η lies in $[-1, 1]$. It is clear that the best possible accuracy will be obtained by integrating the first term on the right-hand side of (6) using a quadrature formula of highest precision with respect to the weight function $(1 - x)^k$ over $[-1, 1]$. The abscissae, x_j, of this quadrature formula are simply the roots of the Jacobi polynomial $P_m^{(k,0)}(x)$ (Krylov [4]) and the weights H_j are given by

$$H_j = \frac{2^{k+1}}{(1 - x_j)^2 [P_m'^{(k,0)}(x_j)]^2} \,. \tag{8}$$

The resulting quadrature formula (7) has degree $2m + k - 1$ and uses $m + k$ functional evaluations. For the same integrating degree (7) uses about $k/2$ more functional evaluations than (2). Tables of the abscissae x_j and weights H_j have been given by Stroud & Secrest [5] for $k = 1$ using 2(1)30 points and for $k = 2$, 3 and 4 using 2(1)20 points.

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