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

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

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

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

where \([x]\) denotes the largest integer \(\leq x\). 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

\[
\int_{0}^{1} \left(\int_{0}^{x} g(x)dx\right)^{n+1} = \frac{1}{n!} \int_{0}^{1} (1 - x)^{n+1}g(x)dx
\]

where \(\left(\int_{0}^{x} g(x)dx\right)^{n}\) denotes repeated integration over \([0, x]\).

It is equally true that

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\[
\int_{-1}^{1} \left( \int_{-1}^{x} g(x)(dx) \right)^{n+1} = \frac{1}{n!} \int_{-1}^{1} (1-x)^n g(x) dx.
\]

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

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

Thus using (4) gives,

\[
\int_{-1}^{1} f(x)dx = \frac{1}{k!} \int_{-1}^{1} (1-x)^k f^{(k)}(x) \left( -x \right) dx + \sum_{i=0}^{k-1} \frac{2^{i+1}}{(i+1)!} f^{(i)}(-1)
\]

\[
= \frac{1}{k!} \sum_{j=1}^{m} H_j f^{(k)}(x_j) + \sum_{i=0}^{k-1} \frac{2^{i+1}}{(i+1)!} f^{(i)}(-1)
\]

\[
+ \frac{2^{k+2m+1}}{(k+2m+1)(2m)!} \left[ \frac{m!(k+m)!}{(k+2m)!} \right]^{2} \int_{-1}^{1} f^{(2m+k)}(\eta) d\eta.
\]

In the remainder term \( \eta \) 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

\[
H_j = \frac{2^{k+1}}{(1-x_j)^2 \left[ P_{m}^{(k,0)}(x_j) \right]^2}.
\]

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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