Quadrature Formulas for Infinite Integrals

By W. M. Harper

1. Introduction. Since the advent of high-speed computers, "mechanical" quadratures of the type

$$\int_a^b w(x)f(x)\,dx \sim \sum_{j=1}^{n} H_j f(a_j) \tag{1}$$

have become increasingly important. The only quadrature generally available for the case $b = -a = \infty$ is the Hermite-Gauss formula although the Laguerre-Gauss formula can also be used if $f(x)$ is an even function of x. The latter would, however, require computation of twice the number of ordinates for a corresponding degree of precision and would therefore rarely be preferred. In either case the integrand is supposed to behave like the product of an exponential function and a polynomial. For purely algebraic integrands it would appear to be more appropriate to use a quadrature based on an algebraic weight function even though the degree of the polynomial approximation to $f(x)$ is limited.

In this paper, formulas of type (1) are derived with weight function $w(x) = (1 + x^2)^{-k-1}$ for the range $b = -a = \infty$. In a modified form they are shown to be superior to the Hermite-Gauss and Laguerre-Gauss quadratures for a particular class of statistical integrals.

2. Derivation of Quadratures. In the quadrature formula

$$\int_{-\infty}^{\infty} (1 + x^2)^{-k-1} f(x)\,dx = \sum_{j=1}^{n} H_j f(a_j) + E_{n,k}, \tag{2}$$

the abscissas a_j will be the zeros of the nth degree polynomial $\phi_{n,k}(x)$ which satisfies the orthogonality condition

$$\int_{-\infty}^{\infty} (1 + x^2)^{-k-1}\phi_{m,k}(x)\phi_{n,k}(x)\,dx = 0, \qquad (m \neq n,\ m + n < 2k + 1). \tag{3}$$

By standard methods given for example in [2], [4], it is easily shown from (3) that the orthogonal system of polynomials is given by the Rodrigues formula

$$\phi_{n,k}(x) = (-1)^n \frac{\Gamma(2k - 2n + 2)}{\Gamma(2k - n + 2)} (1 + x^2)^{k+1} \frac{d^n}{dx^n} (1 + x^2)^{n-k-1}, \qquad (n < k + 1) \tag{4}$$

where the standardizing constant is chosen to make the coefficient of x^n unity. By direct manipulations with (4) and repeated use of Leibnitz' formula, the recurrence relations (5)–(10) are easily established. They are

$$\phi_{n+1,k}(x) = x\phi_{n,k}(x) - \frac{n(2k - n + 2)}{(2k - 2n + 1)(2k - 2n + 3)} \phi_{n-1,k}(x), \tag{5}$$

$$(1 + x^2)\phi'_{n,k}(x) = (2k - n + 1)x\phi_{n,k}(x) - (2k - 2n + 1)\phi_{n+1,k}(x), \tag{6}$$

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$$(7)\qquad (1+x^2)\phi'_{n,k}(x) = nx\phi_{n,k}(x) + \frac{n(2k-n+2)}{2k-2n+3}\phi_{n-1,k}(x),$$

$$(8)\qquad \begin{aligned}\phi_{n,k+1}(x) = {} & \frac{2k-2n+3}{(2k-n+2)(2k-n+3)} \\ & \cdot[\{(4k-2n+3)+(2k-2n+1)x^2\}\phi_{n,k}(x) \\ & -(2k-2n+1)(1+x^2)\phi_{n,k-1}(x)],\end{aligned}$$

$$(9)\qquad \begin{aligned}x(1+x^2)\phi'_{n,k}(x) = {} & [nx^2-(2k-n+2)]\phi_{n,k}(x) \\ & + \frac{(2k-n+2)(2k-n+3)}{2k-2n+3}\phi_{n,k+1}(x),\end{aligned}$$

$$(10)\qquad x\phi'_{n,k}(x) = (2k-n+1)\phi_{n,k}(x) - (2k-2n+1)\phi_{n,k-1}(x).$$

The polynomial system can now be extended to include values of n excluded in (4). For $n > k + \frac{3}{2}$ however, complex zeros make their appearance so that no useful quadratures are available for this range of n.

It is similarly easily shown that $\phi_{n,k}(x)$ is a solution of the differential equation

$$(11)\qquad (1+x^2)y'' - 2kxy' + n(2k-n+1)y = 0$$

whence the relation

$$(12)\qquad \phi_{n,k}(x) = \left(\frac{i}{2}\right)^n n!\,\frac{\Gamma(k-n+\frac{3}{2})}{\Gamma(k+\frac{3}{2})}\,C_n^{-k-1/2}(ix)$$

can be established where in the notation of [1], $C_n^{\lambda}(z)$ (designated by $P_n^{(\lambda)}(z)$ in [7]) is the Gegenbauer or ultraspherical polynomial of degree n and parameter λ. Relations with Legendre functions can also be established, namely:

$$(13)\qquad \begin{aligned}\phi_{n,k}(x) = {} & (-1)^{n+1}\pi^{1/2}\lim_{s\to k} \\ & \cdot\left[2^{s-n}i^{s+n+1}\,\frac{\Gamma(s-n+\frac{3}{2})}{\Gamma(2s-n+2)}\operatorname{cosec} s\pi(1+x^2)^{s/2+1/2}P_{s-n}^{s+1}(ix)\right]\end{aligned}$$

where $P_\nu^\mu(z)$, in the notation of [1], is the associated Legendre function of the first kind with parameters μ and ν, and

$$(14)\qquad \phi_{n,k}(x) = 2^{k-n+1/2}\Gamma(k-n+\tfrac{3}{2})(1+x^2)^{k/2+1/4}\mathrm{P}_{k+1/2}^{-k+n-1/2}[x(1+x^2)^{-1/2}]$$

where $\mathrm{P}_\nu^\mu(z)$ is the associated Legendre function of the first kind with definition suitable for the cut in the real axis from $z = -1$ to $z = 1$. The limit in (13) caters to integer values of k (see [3]).

The weight coefficients and error term in (2) can be determined by standard methods with the results

$$(15)\qquad H_j = 2^{2k-2n+2}n!\,\frac{[\Gamma(k-n+\frac{3}{2})]^2}{\Gamma(2k-n+2)}(1+a_j^2)^{-1}[\phi'_{n,k}(a_j)]^{-2},$$

$$(16)\qquad \begin{cases} E_{n,k} = \dfrac{f^{(2n)}(\xi)}{(2n)!}\displaystyle\int_{-\infty}^{\infty}(1+x^2)^{-k-1}[\phi_{n,k}(x)]^2\,dx \\ \qquad = \dfrac{2^{2k-2n+2}n![\Gamma(k-n+\frac{3}{2})]^2}{(2k-2n+1)(2n)!\Gamma(2k-n+2)}f^{(2n)}(\xi), \qquad \left(n < k+\dfrac{1}{2}\right). \end{cases}$$

The restriction on n is necessary to ensure convergence of the error estimate but does not ensure that a close upper bound to the actual error can be obtained (see, for example, [2]).

For practical purposes a more convenient form of the quadrature is

$$\int_{-\infty}^{\infty} f(x)\,dx \sim \sum_{j=1}^{n} K_j f(a_j); \tag{17}$$

here the weight coefficients are given by

$$K_j = H_j(1 + a_j^2)^{k+1}. \tag{18}$$

The values of a_j and K_j for four- and six-point formulas for some integral values of k are given in Table 1.

The right-hand side of (17) is a function of k as well as of n; for a given value of n, therefore, there will be a value or values of k depending on $f(x)$ which will give the "best" approximation to the integral on the left. The determination of such values and the corresponding parameters appears to be too formidable a task for practical applications. For the special cases $k = n - 1$, $k = n$, however, solution of (11) with $x = \cot\theta$ enables $\phi_{n,k}(x)$ to be obtained in the forms

$$\phi_{n,n-1}(x) = \operatorname{cosec}^n(\operatorname{arc\,cot} x)\cos(n \operatorname{arc\,cot} x), \tag{19}$$

$$\phi_{n,n}(x) = (n + 1)^{-1}\operatorname{cosec}^{n+1}(\operatorname{arc\,cot} x)\sin[(n + 1)\operatorname{arc\,cot} x]. \tag{20}$$

The zeros are now simple cotangents and the weight coefficients H_j assume simple trigonometric form; the resulting quadratures can be written as

$$\int_{-\infty}^{\infty} (1 + x^2)^{-1} f(x)\,dx \sim \frac{\pi}{n}\sum_{j=1}^{n} f\left[\cot\frac{(2j-1)\pi}{2n}\right], \qquad (k = n - 1), \tag{21}$$

$$\int_{-\infty}^{\infty} (1 + x^2)^{-1} f(x)\,dx \sim \frac{\pi}{n+1}\sum_{j=1}^{n} f\left(\cot\frac{j\pi}{n+1}\right), \qquad (k = n). \tag{22}$$

These formulas can also be deduced from the Chebyshev-Gauss quadratures

$$\int_{-1}^{1} (1 - y^2)^{-1/2} g(y)\,dy \sim \frac{\pi}{n}\sum_{j=1}^{n} g\left[\cos\frac{(2j-1)\pi}{2n}\right], \tag{23}$$

$$\int_{-1}^{1} (1 - y^2)^{-1/2} g(y)\,dy \sim \frac{\pi}{n+1}\sum_{j=1}^{n} g\left(\cos\frac{j\pi}{n+1}\right) \tag{24}$$

by the substitutions $y = x(1 + x^2)^{-1/2}$, $g(y) = f(x)$.

3. Practical Application. An example of a useful application for the quadratures is the evaluation of integrals arising in the determination of the statistical distribution of the ratio of two quadratic forms in normal variates. If the quadratic forms are independent mean half-square successive differences based on sample sizes of p and q respectively, one of the integrals which require evaluation can be written in the form

$$I(z) = \int_{-\infty}^{\infty} (1 + x^2)^{-1} \prod_{r=2}^{p-1} (a_r^2 + x^2)^{-1/2} \prod_{s=1}^{q-1} (1 + b_s^2 z^{-1} + x^2)^{-1/2}\,dx, \qquad (p \text{ even}), \tag{25}$$

TABLE 1

Abscissas and Weights for Quadrature (17)

A. $n = 4$

k	$\pm a_j$	K_j
3	0.41421 35624	0.92015 11845
	2.41421 35624	5.36303 41227
4	0.32491 96962	0.69465 18830
	1.37638 19205	1.81862 22399
5	0.27618 30252	0.58086 65620
	1.06005 79874	1.17945 11502
6	0.24436 83118	0.50932 47880
	0.89298 76737	0.90816 46087
7	0.22150 78137	0.45903 94023
	0.78587 59159	0.75578 97944
8	0.20405 97869	0.42121 27662
	0.70979 86678	0.65698 70999
9	0.19017 76238	0.39142 46836
	0.65220 46710	0.58705 73261
10	0.17879 14705	0.36717 90805
	0.60665 77372	0.53455 96626

B. $n = 6$

k	$\pm a_j$	K_j
5	0.26794 91924	0.56119 14763
	1.00000 00000	1.04719 75512
	3.73205 08076	7.81638 89333
6	0.22824 34744	0.47217 91694
	0.79747 33889	0.73421 88392
	2.07652 13966	2.38399 35955
7	0.20219 80919	0.41550 76425
	0.68370 47228	0.58969 00381
	1.57850 04858	1.44716 80133
8	0.18342 80037	0.37535 93234
	0.60816 30047	0.50404 67421
	1.31884 38384	1.06492 43997
9	0.16907 35256	0.34499 40643
	0.55326 32106	0.44635 57833
	1.15411 46518	0.85743 60559
10	0.15763 63749	0.32098 68394
	0.51101 94490	0.40432 69556
	1.03809 74230	0.72680 65190

TABLE 2
Comparison of Quadrature Formulas in Evaluating $I(1)$

Quadrature	No. Abscissas	Result	$E \times 10^8$
Series	—	1.2106 5423	—
Algebraic, $k = 5$	6	1.2106 4384	1039
Algebraic, $k = 6$	6	1.2106 5381	42
Algebraic, $k = 7$	6	1.2106 5415	8
Algebraic, $k = 8$	6	1.2081 0423	25 5000
Algebraic, $k = 9$	6	1.2025 0816	81 4607
Algebraic, $k = 10$	6	1.1942 4044	164 1379
Hermite	6	1.1610 8623	495 6800
Hermite	8	1.1879 0738	227 4685
Hermite	10	1.1994 3337	112 2086
Laguerre	6	1.1674 2007	432 3416

where the a_r and b_s are constants. In order to compare methods (25) was evaluated by various quadratures for the case $p = 4$, $q = 3$, $z = 1$ when the test integral becomes

$$I(1) = \int_{-\infty}^{\infty} (1 + x^2)^{-1} \left[\left(\frac{1}{2}\sqrt{2} + x^2 \right) (2\sqrt{2} - 2 + x^2) \cdot \left\{ \frac{1}{3}(7 - 2\sqrt{2}) + x^2 \right\} \left\{ \frac{1}{9}(13 - 2\sqrt{2}) + x^2 \right\} \right]^{-1/2} dx. \tag{26}$$

The quadrature (17) was applied for the values $k = 5(1)10$ using six abscissas in each case. The Hermite-Gauss quadrature was used with six, eight and ten abscissas, and the Laguerre-Gauss formula for six abscissas (which requires the same number of evaluations of the integrand as the other formulas for twelve abscissas but which is of degree of precision eleven as against twenty-three for the others). The abscissas and weights for the Hermite formula were taken from the values tabulated in [6] and those for the Laguerre method from [5]. The results together with the correct value of $I(1)$ determined by a series method are tabulated to eight decimal places in Table 2 which also shows the errors of the methods.

The table shows the superiority of the "algebraic" quadratures over the Hermite and Laguerre formulas for this integral; even the use of ten abscissas for the Hermite quadrature leaves an error much greater than the algebraic quadratures with only six abscissas except for the case $k = 10$. The best algebraic quadrature is for $k = 7$ but the advantage over those for $k = 5$ and $k = 6$ is too small to compensate for the simplicity of the latter two cases when used in the equivalent forms shown in (21) and (22) respectively. In addition, the quadrature (22) evaluates $I(1)$ correctly to eight decimal places for $n = 8$ as does (21) for $n = 9$.

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