

Abscissas, Coefficients, and Error Term for the Generalized Gauss-Laguerre Quadrature Formula Using the Zero Ordinate

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1. Introduction. Several tables of abscissas and coefficients for the generalized Gauss-Laguerre quadrature formula not using the zero ordinate have been issued recently [1–5]. Such formulas are all of odd degree of precision, and the error term is known [2]. Formulas using the zero ordinate are of even degree of precision; abscissas and coefficients have been tabulated only very briefly by Burnett [6] and copied by Kopal [7], and more elaborately but only for $s = 0$ by Krylov and Fedenko [8]; no formula for the error term has been published—it is derived in Section 3 below.

Table I in Section 2 gives abscissas and coefficients for $s = 0, -1/3, -1/2, -2/3$, with $n = 2(1)16$, thus complementing three of the tables of [2] and [3] by providing the abscissas and coefficients for the quadratures of even degree of precision. A less accurate table covering

$$s = -.99(.01) \quad -.90, -.80, -.75, -.70(.1) \quad -.3, -.25, -.2, -.1, 0(1)10$$

may be obtained by requesting reference [9]. All the tables include values of $H_n e^{ax}$ for convenience in the integration of functions not explicitly containing the factor e^{-x} .

In selecting a formula for practical use in numerical integration one is usually concerned with two matters: (1) a minimum amount of calculational labor and (2) an error which is acceptably small. The amount of calculational labor often is controlled by the number of times that $f(x)$ must be evaluated, and the only significant difference between one evaluation and another is that $f(0)$ may be zero or more easily calculated than other values. If the labor of calculating $f(0)$ may be neglected, the number of evaluations of $f(x)$ for the formula using the zero ordinate and of degree of precision $2n - 2$ is $n - 1$, the same as the number of evaluations for the formula not using the zero ordinate and of lower degree of precision $2n - 3$; otherwise the number of evaluations is n and equals that not using the zero ordinate of degree of precision $2n - 1$. Anticipating the result of Section 3, we see that the error terms of the degrees of precision $2n - 3, 2n - 2$ and $2n - 1$ are, respectively,

$$\frac{(n-1)! \Gamma(n+s)f^{(2n-2)}(\eta)}{(2n-2)!}, \quad \frac{(n-1)! \Gamma(n+s+1)f^{(2n-1)}(\eta)}{(2n-1)!},$$
$$\frac{n! \Gamma(n+s+1)f^{(2n)}(\eta)}{(2n)!}.$$

Disregarding the unknown behavior of the higher derivatives, the ratio of the second coefficient to the first is $(n+s)/(2n-1)$; the ratio of the third coefficient

to the second is $1/2$. Thus, for the values of n and s included in Table I, the first ratio is nearly $1/2$; the error terms decrease in a uniform way; if the labor to evaluate $f(0)$ is negligible, one should select the formula with the zero ordinate, otherwise use the formula with the same number of ordinates not including $x = 0$. For the larger values of s , such as some of those in reference [9], the first ratio becomes larger than 1, and the selection of a most suitable formula cannot be stated so simply.

2. Numerical Values of Abscissas and Coefficients. The abscissas a_j and the coefficients H_j , given in Table I following are derived from the requirement of maximum degree of precision ($E = 0$ for $f(x)$ a polynomial of as high degree as possible) of the quadrature formula

$$(1) \quad \int_0^\infty x^s e^{-x} f(x) dx = H_1 f(0) + \sum_{j=2}^n H_j f(a_j) + E.$$

Since the a_j and H_j , including H_1 but excluding $a_1 = 0$, constitute a set of $2n - 1$ parameters, the degree of precision is $2n - 2$.

Numerical values have been calculated by using the formulas given by Kopal [7]. Equivalent formulas may be found in Mineur [10] and in Krylov and Fedenko [8]. (Facile comparison of formulas and numerical values is impeded by differences of notation. E. g., Kopal's H_1 does not include the factor $1 + s$ which is included by Krylov and Fedenko and in formula (1) herein; Krylov and Fedenko begin formula (1) with $Af(0)$ and run the summation from 1 to n so that their n is one smaller than the present n which is the same as Kopal's.) Krylov and Fedenko [8] have observed that the $a_j \neq 0$ of (1) are the same as the a_j of the formula not using the zero ordinate, but for a value of s increased by unity:

$$\int_0^\infty x^{s+1} e^{-x} f(x) dx = \sum_{j=2}^n K_j f(a_j)$$

and that $K_j = H_j a_j$ ($j = 2, \dots, n$).

The abscissas of (1) are roots of the polynomial

$$(2) \quad \Lambda_n^s(x) \equiv L_n^s(x) - (n + s)L_{n-1}^s(x) = 0,$$

where $L_n^s(x)$ represents the generalized Laguerre (or Sonine) polynomial. As given in [7],

$$H_j = \frac{\Gamma(n)\Gamma(n+s)}{(n+s)\{L_{n-1}^s(a_j)\}^2},$$

but the present notation incorporates the factor $1 + s$ into H_1 .

For each combination of n and s , the accuracy of calculated a 's and H 's has been checked by the relations

$$\sum_{j=1}^n a_j = (n-1) \cdot (n+s), \quad \prod_{j=2}^n a_j = \frac{\Gamma(n+s+1)}{\Gamma(s+2)} \quad \text{and} \quad \sum_{j=1}^n H_j = \Gamma(s+1).$$

In no case do the calculated and theoretical values differ in more than the last two digits. Since there are obvious cases (e.g., H_1 at $s = 0, n = 11$) in which the calculated values are incorrect in the last two digits, it is expected that only 14 digits of H are reliable. The a 's are probably good to 15 digits.

TABLE I (continued)

S=-1/3		S=2/3	
N	A	H X EXP(A)	H X EXP(A)
14	0.0000000000000000 00	2.1211375504046780-01	1.0005098363608250 00
	6.5540334970127650-01	1.0000000000000000 00	1.0005098363608250 00
	8.1671233773874650-01	0.5423000000000000 00	0.5423000000000000 00
	9.33914503841842350-01	6.68336566920040200-01	6.68336566920040200-01
	1.04453153871624550-00	1.55379350559580 00	1.694152664856720-01
	1.1426675404291940 00	2.82166206591950 00	4.27226446224660-02
	1.25621326719150-00	4.48950813459974 00	7.44951734318696 03
	1.356276710973740 00	9.1564873891039890 00	6.61505529451623 00-01
	1.46703071210180-04	1.016998800210180-04	6.8055337672336800 04
	1.8228522828890-06	1.22606229997530 00	6.4371312525366610 05
	1.6358186483114730-01	1.2606483114730-01	6.35183546607893 00-01
	2.08154996122775310 01	1.61618802656299740 00	6.3615122798690650-08
	2.6200888957675050 01	1.7705191604390 00	6.487339949196720-01
	3.299489755494720 01	2.005871176121690 00	6.7838955118249-01
4.1927327655762540 01	2.370719875928450 00	3.234191915871510 01	7.43838648020360-15
	3.16653393770805840 00	4.13268906226714070 01	9.1561613347728130-01
15	0.0000000000000000 00	2.024722072044670-01	9.7722157777310-01
	5.1691013181507646-01	6.225418845320200-01	9.7582295521760-01
	7.21573367594459198-01	7.893930511264670-01	4.80800849823230-01
	1.5925235692143830 00	6.44382019685934713-01	4.8397018064240-01
	2.81157627063130 00	9.5958461306498730-01	1.4452124645746437 00
	4.4040428375206930 00	1.3270000000000000 00	2.621784746409960 00
	6.382823264234990 00	1.9824245588257180-03	4.167501775019940 00
	8.7709614426270190 00	1.9557887399133580-04	6.1036871758077650 00
	1.1652488932030520 01	1.2117836901572660-05	6.143087504677860 00
	1.50083775429260 01	4.49730396844930-05	6.127616420103670 01
	1.891976505217220 01	9.3383884875189380 00	1.460998930622900 01
	2.36716265946970220 01	1.6150198424858220-11	2.320088737024390 01
	3.0250432502220 01	2.70718702821090-13	2.87094224108730 01
	3.6265533759374990 01	4.222848661268220 00	3.5709567069820 01
4.555761378575620 01	5.0932451568670430-20	3.1696828088381670 00	4.4970306369566460 01
16	0.0000000000000000 00	1.9385638154085330-01	9.5599777084022260-01
	1.8000106433759810-01	5.9817300925653463-01	9.6326622799800150-01
	6.7567126890467700-01	3.79152545943200-01	1.3451573379819630-01
	3.79152545943200-01	5.98165815059630-01	1.3515112302056900 00
	8.5457141192910440-01	9.4807950818723165-01	1.44929192337440 00
	9.4807950818723165-01	1.03377955718840 00	3.8895981581982650 00
	1.695253401897930-02	2.90525305254500-03	5.68780265921933 00
	1.1162997068163590 00	3.405214161231360 00	2.10931246354792 03
	1.079333941674780 01	2.6399972883774900-04	2.304584212136390 04
	1.388343802967010 01	1.299115585842450 00	1.6840000555528460 05
	1.492204151676160-08	1.383160114322890 00	5.8788638016235350-01
	2.63157633002468090 00	1.922387948777990-01	4.8642317397781320-01
	4.11277885502454460 00	6.828477663409090-02	1.9735557589711630-01
	5.95087726815120 00	1.695253401897930-02	6.0154558885674750 02
	8.1612997068163590 00	1.1162997068163590 00	1.336172211920320 01
	1.079333941674780 01	1.20068005595910360 00	2.10931246354792 03
	1.388343802967010 01	1.288864305857490 00	2.304584212136390 04
	1.492204151676160-08	1.383160114322890 00	1.6840000555528460 05
	2.1675449851173850 01	6.27020501311220 00	5.805434281114140-01
	2.6556115954172390 01	5.032916210223340 00	5.7966466815401070 01
	3.2447778916865250 01	2.015251924338840 00	3.863348687224040 01
	3.965719950949550 01	1.42202563882190-17	6.2757055987261140-12
4.9242593715633410 01	1.301151156415830-18	3.1724622137456430 00	6.6138615319471180-15
		4.4970306369566460 01	7.35857361723599816-18
		5.8655824685112550 01	8.68957361723599816-22

For $s = 0$, comparison with the 8-place tables of [8] discloses that 17 of 240 entries therein are incorrect in the 8th digit, presumably due to rounding, and 4 cases (in their notation: A_2 of $n = 6$, A_3 of $n = 12$, A_{12} of $n = 14$, X_{15} of $n = 15$) of misprints or errors. Among the 24 possible comparisons with $s = 1$ of [1], there are 5 cases in which, rounding their a 's to 16 figures, our last digits are in error by 1 unit; there are 4 cases in which their weights and our $a_j \cdot H_j$ differ by one when rounded to 14 digits. Since reference [5] is known to the author only via Mathematical Reviews, comparison with it cannot be made.

3. The Error Term. Since published formulas do not include that for the error term, this term is derived below, some of the essential ideas being found in [6].

If $f(x)$ is a polynomial of degree $2n - 2$ or less, it can be written

$$(3) \quad f(x) = \Lambda_n^s(x) \cdot \sum_{r=0}^{n-2} A_r \Lambda_r^s(x) + \sum_{k=1}^n B_k \frac{\Lambda_n^s(x)}{x - a_k}$$

where $\Lambda_0^s(x) = 1$ and the B 's are to be evaluated from

$$(4) \quad f(a_j) = B_j \left[\frac{d}{dx} \Lambda_n^s(x) \right]_{x=a_j} \quad j = 1, \dots, n$$

and the A 's are to be determined from the requirements

$$(5) \quad f'(a_j) = \left[\frac{d}{dx} \Lambda_n^s(x) \right]_{x=a_j} \cdot \sum_{r=0}^{n-2} A_r \Lambda_r^s(a_j) + \sum_{k=1, k \neq j}^n (B_k + B_j) \cdot \frac{\Lambda_n^s(x)}{(x - a_j)(x - a_k)} \Big|_{x=a_j} \quad (j = 2, \dots, n).$$

Thus the left and right members of (3) are polynomials of degree $2n - 2$ or less coinciding at the n points $x = a_j$ and with equal derivatives at $n - 1$ points $x = a_j \neq 0$, hence are identical.

If $f(x)$ is not a polynomial of degree $2n - 2$ or less, then (3) will not be exact, but must contain a remainder term:

$$(6) \quad f(x) = \Lambda_n^s(x) \cdot \sum_{r=0}^{n-2} A_r \Lambda_r^s(x) + \sum_{k=1}^n B_k \frac{\Lambda_n^s(x)}{x - a_k} + R_{2n-1}(x)$$

and some form for $R_{2n-1}(x)$ is to be sought. We examine the possibility that

$$(7) \quad R_{2n-1}(x) = K(x) \cdot \frac{[\Lambda_n^s(x)]^2}{x}.$$

Let the right member of (3) be denoted by $\theta(x)$, and consider the function

$$\Phi(x) = f(x) - \theta(x) - R_{2n-1}(x).$$

With A 's and B 's determined by (4) and (5), and with R in the form (7), $\Phi(x)$ has zeros at $x = a_j$ and vanishing first derivative at $x = a_j \neq 0$. Then, selecting some arbitrary $x = \bar{x}$ different from all a_j , $K(\bar{x})$ can be determined so that $\Phi(\bar{x}) = 0$. Then $\Phi(x)$ has double zeros at $x = a_j$ ($j = 2, \dots, n$) and simple zeros at $x = 0$ and $x = \bar{x}$. Hence, by $(2n - 1)$ -fold application of Rolle's Theorem,

$$\Phi^{(2n-1)}(\xi) = f^{(2n-1)}(\xi) - K(\bar{x}) \cdot (2n - 1)! = 0 \quad \text{for some } \xi.$$

This permits writing the remainder term in the form

$$R_{2n-1}(x) = \frac{f^{(2n-1)}(\xi)}{(2n-1)!} \frac{[\Lambda_n^s(x)]^2}{x}, \quad 0 \leq \xi \leq \max(a_j, \bar{x}).$$

When (6) is substituted into the left member of (1), the terms of the first summation vanish because they are orthogonal with respect to the weight function; the terms of the second summation become the nonremainder terms of the right member; the integral of $R_{2n-1}(x)$ becomes E as follows:

$$\begin{aligned} E &= \int_0^\infty x^s e^{-x} \frac{f^{(2n-1)}(\xi)}{(2n-1)!} \frac{[\Lambda_n^s(x)]^2}{x} dx, \quad 0 \leq \xi \leq \max(a_j, x), \\ &= \frac{f^{(2n-1)}(\eta)}{(2n-1)!} \int_0^\infty x^{s+1} e^{-x} \frac{[\Lambda_n^s(x)]^2}{x} dx, \quad 0 \leq \eta \leq \infty, \\ &= \frac{f^{(2n-1)}(\eta)}{(2n-1)!} \int_0^\infty x^{s+1} e^{-x} [\Lambda_{n-1}^{s+1}(x)]^2 dx, \quad 0 \leq \eta \leq \infty, \\ &= \frac{f^{(2n-1)}(\eta)}{(2n-1)!} \cdot (n-1)! \Gamma(n+s+1), \quad 0 \leq \eta \leq \infty. \end{aligned}$$

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