Gaussian Quadratures for the Integrals

$$\int_0^\infty \exp(-x^2)f(x)dx \text{ and } \int_0^b \exp(-x^2)f(x)dx$$

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Abstract. Gaussian quadratures are developed for the evaluation of the integrals given in the title. The weights and abscissae for the semi-infinite integral are given for two through fifteen points with fifteen places. For $b = 1$, the weights and abscissae are given for two through ten points with fifteen places.

1. Introduction. In nuclear reactor design calculations, the evaluation of the effective radiative neutron capture cross-sections from a statistical model of the neutron-target interaction leads to integrals of the form

$$\int_0^b \exp(-x^2)f(x)dx\,, \qquad b < \infty \tag{1.1}$$

and

$$\int_0^\infty \exp(-x^2)f(x)dx\,. \tag{1.2}$$

In such problems, f is undefined for $x < 0$ and difficult to evaluate otherwise. For this reason, Gaussian quadratures for the evaluation of (1.1) and (1.2) are developed and their weights and abscissae are given in Tables II and III. It should be noted that the classical variants of Gauss quadrature are not applicable to (1.1). The integral of (1.2) *can* be transformed so that the Laguerre-Gauss quadrature is applicable. Unfortunately, for the function considered here, the required transformation of variable, $u = x^2$, leads to an integrand that is singular at the origin. Note that (1.2) could, in principle, be evaluated using the Hermite-Gauss quadrature by considering a function, g, which is an even extension of f about the origin. Often, however, g is of low-order differentiability at the origin. When this is true, the resulting approximations to (1.2) obtained by successive Hermite-Gauss quadratures tend to oscillate, with increasing N, about the true solution. This is demonstrated by the data in Table I. These data are Hermite-Gauss quadrature approximations to the integral of (1.2) for $f(x) = x^k$, $k = 1, 3$ using $g(x) = |x|^k$. The exact value of the integral for both cases is $\frac{1}{2}$. The examples shown are for k odd. When k is even, $|x|^k = x^k$ and the Hermite-Gauss quadratures are exact so long as $k \leqq 2N - 1$.

It should be pointed out that if f is an even function the Hermite-Gauss quadratures may converge to (1.2) more rapidly than the quadratures presented in this paper. The reason is that the abscissae of the Hermite-Gauss quadratures are symmetrically distributed about the origin. Thus the evaluation of (1.2) with an M-point Hermite-Gauss quadrature, where M is even, only requires the use of the $N = \frac{1}{2}M$ points on the positive axis. The truncation error term however is still

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of the form $C_M f^{(2M)}(\theta)$ or $C_{2N} f^{(4N)}(\theta)$, $\theta \in [0, \infty)$. The error term for an N-point quadrature of the type developed here is $D_N f^{(2N)}(\theta)$ which involves only the $2N$th derivative while that of the Hermite-Gauss quadrature, also using only N-points contains the $4N$th derivative of f as well as the coefficient, C_M, for the higher-order quadrature.

TABLE I

N	*Hermite-Gauss Approximation*	*Relative Error, %*
	$k = 1$	
2	0.6267	−25.3
3	0.3618	27.6
4	0.5565	−11.3
5	0.4176	16.5
6	0.5365	− 7.3
7	0.4412	11.8
8	0.5269	− 5.4
9	0.4543	9.1
10	0.5213	− 4.3
	$k = 3$	
2	0.3133	37.3
3	0.5427	− 8.5
4	0.4820	3.6
5	0.5112	− 2.2
6	0.4933	1.3
7	0.5051	− 1.0
8	0.4965	0.7
9	0.5030	− 0.6
10	0.4979	0.4

2. Computation of Weights and Abscissae. Since the theory of Gaussian quadrature is well known only the special results for the cases of interest here will be presented. The abscissae, x_j, $j = 1, \cdots, N$ are the zeros of the Nth degree polynomial, $p_N(x)$, orthogonal on the interval of integration with respect to the weight function, $w(x) = \exp(-x^2)$. Because of the similarity of form we will discuss in detail only the case for the finite upper limit, b. The semi-infinite case follows directly by taking the appropriate limits as $b \to \infty$.

The weights of the quadratures are computed from the well-known expression

$$W_j = \gamma_{N-1}/[p_N'(x_j)p_{N-1}(x_j)] , \qquad j = 1, \cdots, N \tag{2.1}$$

which follows from the Christoffel-Darboux identity. The term γ_N is given by

$$\gamma_N = \int_0^b \exp(-x^2) p_N^2(x) dx . \tag{2.2}$$

The orthogonality properties only define the polynomials within an arbitrary multiplicative constant. For convenience the constant has been selected to make the polynomials monic. Thus the first two polynomials are

$$p_0(x) = 1 \,, \tag{2.3}$$

$$p_1(x) = x - [1 - \exp(-b^2)]/[\sqrt{\pi}\,\mathrm{erf}\,(b)] \,. \tag{2.4}$$

The higher-order polynomials were generated from the three term recurrence relation between successive orthogonal polynomials which is of the form

$$p_{k+1}(x) = (x + \alpha_k)p_k(x) + \beta_k p_{k-1}(x) \,, \qquad k = 1, \cdots \tag{2.5}$$

in which the parameters, α_k, β_k, are defined as

$$\alpha_k = -\gamma_k^{-1} \int_0^b \exp(-x^2) x p_k^2(x) dx \,, \tag{2.6}$$

$$\beta_k = -\gamma_k/\gamma_{k-1} \,. \tag{2.7}$$

The polynomials could be generated directly from (2.2)-(2.7), by evaluating the integrals in (2.2) and (2.6) in a straightforward manner. However, the following method of evaluating α_k and γ_k was developed which requires relatively few arithmetic operations. This method is derived below.

Observe that

$$p_k(0) = \alpha_{k-1}p_{k-1}(0) + \beta_{k-1}p_{k-2}(0) \,, \tag{2.8}$$

$$p_k(b) = (b + \alpha_{k-1})p_{k-1}(b) + \beta_{k-1}p_{k-2}(b) \,, \qquad b < \infty \,. \tag{2.9}$$

The orthogonality conditions permit γ_k, of (2.2), to be expressed as

$$\gamma_k = \int_0^b \exp(-x^2) p_k(x) p_{k-1}(x) x dx \tag{2.10}$$

by multiplying (2.5) by $\exp(-x^2)p_{k-1}(x)$ and integrating. This result may then be integrated by parts to obtain

$$\begin{aligned}\gamma_k = &-\frac{1}{2}[\exp(-x^2)p_k(x)p_{k-1}(x)]|_0^b \\ &+ \frac{1}{2}\int_0^b \exp(-x^2)p_k'(x)p_{k-1}(x)dx \,.\end{aligned} \tag{2.11}$$

The integral of (2.11) may be evaluated, using the Christoffel-Darboux identity, as follows. Let

$$Z_{k-1} = \int_0^b \exp(-x^2) p_k'(x) p_{k-1}(x) dx \,. \tag{2.12}$$

From the orthogonality of p it follows that Z_{k-1} may also be expressed as

$$Z_{k-1} = \int_0^b \exp(-x^2)[p_k'(x)p_{k-1}(x) - p_k(x)p_{k-1}'(x)]dx \,. \tag{2.13}$$

An easily derived consequence of the Christoffel-Darboux identity is the relation

$$p_k'(x)p_{k-1}(x) - p_k(x)p_{k-1}'(x) = \gamma_{k-1}\sum_{r=0}^{k-1} p_r^2(x)/\gamma_r \,. \tag{2.14}$$

Multiplication of (2.14) by $\exp(-x^2)$ and integration provides the result

$$Z_{k-1} = k\gamma_{k-1} \,. \tag{2.15}$$

Thus (2.11), together with (2.15), leads to the recurrence relation

$$\gamma_k = \tfrac{1}{2}k\gamma_{k-1} - \tfrac{1}{2}[\exp(-x^2)p_k(x)p_{k-1}(x)]_0^b . \tag{2.16}$$

A recurrence relation may be obtained for α_k upon integration of (2.6) by parts. The result is

$$\alpha_k = \tfrac{1}{2}\gamma_k^{-1}[\exp(-x^2)p_k^2(x)]_0^b . \tag{2.17}$$

The recurrence relation for β_k follows directly from (2.7) using (2.16). With the aid of the above equations, (2.5) provides a completely recursive means of generating the higher-order polynomials.

Since the weight function, $w(x) = \exp(-x^2)$, is nonzero on the interval of integration the zeros of the polynomials are known to be real, distinct and to lie in the interior of the interval. Consequently the zeros were computed numerically using Newton-Raphson iteration, starting with the smallest zero. As each zero was approximated the order of the polynomial was reduced and the smallest zero of the reduced polynomial was approximated. The zeros obtained in this manner were then tested in the original polynomial and corrected as necessary.

The error coefficients, D_N, listed in the following tables are the coefficients of the $2N$th derivative of the function, f, appearing in the standard expression for the truncation error, E_N, defined as

$$E_N = D_N f^{(2N)}(\theta) , \qquad \theta \in [0, b] , \tag{2.18}$$

where D_N is

$$D_N = \gamma_N/(2N)! . \tag{2.19}$$

Quadratures corresponding to values of b from 0.05 through 0.95 in steps of 0.05 have also been generated and tabulated [1] but it would be impractical to attempt to list them here.

In a paper of this sort, it is customary to assess the validity of the weights and abscissae given in Tables II and III by using them in the quadrature analogues of the integrals:

$$\begin{aligned} I_0 &= \int_0^b \exp(-x^2)dx = \tfrac{1}{2}\sqrt{\pi}\,\mathrm{erf}(b) \\ I_1 &= \int_0^b x\exp(-x^2)dx = \tfrac{1}{2}[1 - \exp(-b^2)] \\ &\ \ \vdots \\ I_k &= \int_0^b x^k \exp(-x^2)dx = \frac{(k-1)}{2} I_{k-2} - \frac{1}{2} b^{k-1}\exp(-b^2) \end{aligned} \tag{2.20}$$

for $k = 1, 2, \cdots, 2N - 1$ and comparing these approximate results with the exact results. The data given in Tables II and III were checked by this process and were found to be accurate to six units in the fifteenth place.

This check verifies the accuracy of the data in these tables for the purpose of integration, which is the primary objective in this paper.

TABLE - II

WEIGHTS AND ABSCISSAE OF GAUSSIAN QUADRATURES FOR THE INTERVAL (0,INF.) WITH WEIGHT FUNCTION

$W(X) = EXP(-X^2)$

WEIGHTS	ABSCISSAE
N = 2	
6.40529179684379D-01	3.00193931060839D-01
2.45697745768379D-01	1.25242104533372D+00
ERROR COEF. = 22900-02	
N = 3	
4.46029770466658D-01	1.90554149798192D-01
3.96468266998335D-01	8.48251867544577D-01
4.37288879877644D-02	1.79977657841573D+00
ERROR COEF. = 38545-04	
N = 4	
3.25302999756919D-01	1.33776446996068D-01
4.21107101852062D-01	6.24324690187190D-01
1.33442500357520D-01	1.34253782564499D+00
6.37432348625728D-03	2.26266447701036D+00
ERROR COEF. = 46135-06	
N = 5	
2.48406152028443D-01	1.00242151968216D-01
3.92331066652399D-01	4.82813966046201D-01
2.11418193076057D-01	1.06094982152572D+00
3.32466603513439D-02	1.77972941852026D+00
8.24853344515628D-04	2.66976035608766D+00
ERROR COEF. = 42863-08	
N = 6	
1.96849675488598D-01	7.86006594130979D-02
3.49154201525395D-01	3.86739410270631D-01
2.57259520584421D-01	8.66429471682044D-01
7.60131375840057D-02	1.46569804966352D+00
6.85191862513596D-03	2.17270779693900D+00
9.84716452019267D-05	3.03682016932287D+00
ERROR COEF. = 32548-10	
N = 7	
1.60609965149261D-01	6.37164846067008D-02
3.06319808158099D-01	3.18192018888619D-01
2.75527141784905D-01	7.24198989258373D-01
1.20630193130784D-01	1.23803559921509D+00
2.18922863438067D-02	1.83852822027095D+00
1.23644672831056D-03	2.53148815132768D+00
1.10841575911059D-05	3.37345643012458D+00
ERROR COEF. = 20900-12	

TABLE II (CONTINUED)

N = 8

1.34109188453360D-01	5.29786439318514D-02
2.68330754472640D-01	2.67398372167767D-01
2.75953397988422D-01	6.16302884182402D-01
1.57448282618790D-01	1.06424631211623D+00
4.48141099174625D-02	1.58885586227006D+00
5.36793575602526D-03	2.18392115309586D+00
2.02063649132407D-04	2.86313388370808D+00
1.19259692659532D-06	3.68600716272440D+00

ERROR COEF. = 11626-14

N = 9

1.14088970242118D-01	4.49390308011934D-02
2.35940791223685D-01	2.28605305560535D-01
2.66425473630253D-01	5.32195844331646D-01
1.83251679101663D-01	9.27280745338081D-01
7.13440493066916D-02	1.39292385519588D+00
1.39814184155604D-02	1.91884309919743D+00
1.16385272078519D-03	2.50624783400574D+00
3.05670214897831D-05	3.17269213348124D+00
1.23790511337496D-07	3.97889886978978D+00

ERROR COEF. = 57051-17

N = 10

9.85520975191087D-02	3.87385243257289D-02
2.08678066608185D-01	1.98233304013083D-01
2.52051688403761D-01	4.65201111814767D-01
1.98684340038387D-01	8.16861885592273D-01
9.71984227600620D-02	1.23454132402818D+00
2.70244164355446D-02	1.70679814968913D+00
3.80464962249537D-03	2.22994008892494D+00
2.28886243044656D-04	2.80910374689875D+00
4.34534479844469D-06	3.46387241949586D+00
1.24773714817825D-08	4.25536180636608D+00

ERROR COEF. = 25043-19

N = 11

8.62207055355942D-02	3.38393212320868D-02
1.85767318955695D-01	1.73955727711686D-01
2.35826124129815D-01	4.10873840975301D-01
2.05850326841520D-01	7.26271784264131D-01
1.19581170615297D-01	1.10386324647012D+00
4.31443275880520D-02	1.53229503458121D+00
8.86764989474414D-03	2.00578290247431D+00
9.27141875082127D-04	2.52435214152551D+00
4.15719321667468D-05	3.09535170987551D+00
5.86857646837617D-07	3.73947860994972D+00
1.22714513994286D-09	4.51783596719327D+00

ERROR COEF. = 99447-22

TABLE II (CONTINUED)

N = 12

7.62461468014692D-02	2.98897007730461D-02
1.66446068894088D-01	1.54204878281815D-01
2.19394898138567D-01	3.66143963007318D-01
2.07016508675540D-01	6.50881015894534D-01
1.37264362783550D-01	9.94366869943082D-01
6.05056743380072D-02	1.38589120372088D+00
1.65538019519272D-02	1.81884860850511D+00
2.58608378742107D-03	2.29084273875259D+00
2.06237540974292D-04	2.80409679347421D+00
7.06650986370700D-06	3.36727070424289D+00
7.59131546779026D-08	4.00168347575167D+00
1.18195417081408D-10	4.76821628806517D+00

ERROR COEF. = 36052-24

N = 13

6.80463905352764D-02	2.66511266597122D-02
1.50057211876373D-01	1.37891855649089D-01
2.03606639827325D-01	3.28828675536304D-01
2.04104355193263D-01	5.87378532052256D-01
1.50119228114358D-01	9.01480885282686D-01
7.74536314139415D-02	1.26129650345530D+00
2.64891666492538D-02	1.66003713286282D+00
5.62343028882350D-03	2.09410900519525D+00
6.83241175771430D-04	2.56320702628643D+00
4.24853316505515D-05	3.07091234206554D+00
1.13557100512952D-06	3.62669201282754D+00
9.46453637801777D-09	4.25220740148118D+00
1.11810460611588D-11	5.00800834420412D+00

ERROR COEF. = 12023-26

N = 14

6.12109822716413D-02	2.39567896629936D-02
1.36062060620609D-01	1.24240346144723D-01
1.88856803527084D-01	2.97338573288085D-01
1.98577829123488D-01	5.33329221273305D-01
1.58617337872050D-01	8.21873198117369D-01
9.28167828948399D-02	1.15406708458062D+00
3.79316390125047D-02	1.52327480337614D+00
1.02563910691812D-02	1.92533822320942D+00
1.72277180701059D-03	2.35860077983781D+00
1.65956340534487D-04	2.82409376823402D+00
8.19589322531928D-06	3.32626937208736D+00
1.73876608495078D-07	3.87510500420455D+00
1.14293978310768D-09	4.49243808452490D+00
1.04120010017399D-12	5.23843137515097D+00

ERROR COEF. = 37125-29

TABLE II (CONTINUED)

N = 15

5.54433663102343D-02	2.16869474675590D-02
1.24027738987730D-01	1.12684220347775D-01
1.75290943892075D-01	2.70492671421899D-01
1.91488340747342D-01	4.86902370381935D-01
1.63473797144070D-01	7.53043683072978D-01
1.05937637278492D-01	1.06093100362236D+00
5.00270211534535D-02	1.40425495820363D+00
1.64429690052673D-02	1.77864637941183D+00
3.57320421428311D-03	2.18170813144494D+00
4.82896509305201D-04	2.61306084533352D+00
3.74908650266318D-05	3.07461811380851D+00
1.49368411589636D-06	3.57140815113714D+00
2.55270496934465D-08	4.11373608977209D+00
1.34217679136316D-10	4.72351306243148D+00
9.56227446736465D-14	5.46048893578335D+00

ERROR COEF. = 10672-31

TABLE - III

WEIGHTS AND ABSCISSAE OF GAUSSIAN QUADRATURES FOR THE INTERVAL (0,1.00) WITH WEIGHT FUNCTION

$W(X) = EXP(-X^2)$

N = 2

WEIGHTS	ABSCISSAE
4.31325364170332D-01	1.89608043270740D-01
3.15498768642095D-01	7.42562394488043D-01

ERROR COEF. = 15778-03

N = 3

WEIGHTS	ABSCISSAE
2.53700192457267D-01	1.04475414746960D-01
3.43144645828844D-01	4.65591332333112D-01
1.49979294526316D-01	8.65383946240150D-01

ERROR COEF. = 33976-06

N = 4

WEIGHTS	ABSCISSAE
1.63034604989450D-01	6.55295245474369D-02
2.79934755021517D-01	3.10558620696937D-01
2.18855584041643D-01	6.41085413223258D-01
8.49991887598173D-02	9.19249071295932D-01

ERROR COEF. = 38580-09

N = 5

WEIGHTS	ABSCISSAE
1.12646511369676D-01	4.47677711283395D-02
2.16681115495002D-01	2.19457476213530D-01
2.20720515248768D-01	4.77801751524747D-01
1.42441764830179D-01	7.48160820317653D-01
5.43342258688018D-02	9.46641977439054D-01

ERROR COEF. = 27081-12

TABLE III (CONTINUED)

N = 6

8.21931584888009D-02	3.24661014738995D-02
1.68093171657335D-01	1.62403791544834D-01
1.97728490064862D-01	3.65192922556895D-01
1.63278375115819D-01	5.99091843952587D-01
9.78718350596067D-02	8.15631492565660D-01
3.76591024260037D-02	9.62255559768127D-01

ERROR COEF. = 12917-15

N = 7

6.25065724477524D-02	2.45998022135265D-02
1.32553267408311D-01	1.24654588269490D-01
1.69774770042795D-01	2.86306147073804D-01
1.62429751086312D-01	4.83616811726703D-01
1.21152909496289D-01	6.86019406453583D-01
7.07790189509976D-02	8.60030242686043D-01
2.76278433799691D-02	9.71939583327556D-01

ERROR COEF. = 44594-19

N = 8

4.90882051189123D-02	1.92734192234665D-02
1.06525203671690D-01	9.85176987436895D-02
1.43947177209678D-01	2.29598292416142D-01
1.51307979402994D-01	3.95651061416866D-01
1.29555768236386D-01	5.76297029050948D-01
9.18762308512729D-02	7.49083984906103D-01
5.33903928573824D-02	8.90484489455275D-01
2.11331754641105D-02	9.78340479473957D-01

ERROR COEF. = 11660-22

N = 9

3.95488165784004D-02	1.55030326457613D-02
8.71639032969965D-02	7.97311964871323D-02
1.22038930369815D-01	1.87762530384973D-01
1.36601850815752D-01	3.28226061703989D-01
1.28434308712960D-01	4.87018253938628D-01
1.03227785327047D-01	6.48410556244687D-01
7.14613562927916D-02	7.95713083865440D-01
4.16580238804577D-02	9.12151359102553D-01
1.66891575382076D-02	9.82784590735890D-01

ERROR COEF. = 23892-26

TABLE III (CONTINUED)

N = 10

3.25319695101801D-02	1.27378499713740D-02
7.24838964037449D-02	6.58023279743935D-02
1.04004662155270D-01	1.56155783059660D-01
1.21594475562980D-01	2.75890718366863D-01
1.22093608318116D-01	4.14966322218475D-01
1.07195747923389D-01	5.62009142193357D-01
8.30779890294863D-02	7.04832804690269D-01
5.69285988401857D-02	8.30893869740303D-01
3.33982919934992D-02	9.28057569743495D-01
1.35148930755755D-02	9.85992766817013D-01

ERROR COEF. = 39397-30

TABLE IV

Approximate Error Amplification Factors of Relation (2.16)

Upper integration limit	$n = 5$	$n = 10$	$n = 15$
∞	10^3	10^5	10^7
1.0	10^7	10^{15}	—

It should be pointed out, however, that this check does not insure the accuracy of the individual weights and abscissae in Tables II and III to the number of places cited. Since the abscissae in Table II are the zeros of the half-range Hermite polynomials they alone may be of interest to some readers. The accuracy of the individual entries may be estimated by examining the stability of the algorithm.

The primary instability of the algorithm presented in this paper is in the recursive evaluation of γ_n using Eq. (2.16). The significance of this instability may be examined using the analysis developed by Gautschi [2] as follows. Suppose a relative error, ϵ, is introduced in the computation of γ_0. This may be rounding error for example. Consider now the propagation of this error throughout the sequence $\{\gamma_1, \gamma_2, \cdots, \gamma_n\}$ via the recurrence relation. For simplicity, assume that all other computations are carried out with infinite precision. Gautschi has shown that the relative error in γ_n is then $\rho_n \epsilon$ where the amplification factor, ρ_n, is given by Eq. (2.21)

$$(2.21) \qquad \rho_n = \gamma_0 h_n / \gamma_n \, .$$

In the case at hand, h_n is expressed as

$$(2.22) \qquad h_n = \prod_{k=0}^{n-1} \left(\frac{k+1}{2} \right) = n!/2^n \, .$$

If ρ_n is greater than 1, the initial error is amplified throughout the sequence. Table IV contains some approximate values of ρ_n related to Eq. (2.16).

All the data given here were computed in double-precision arithmetic on the CDC-6600 computer, which provides a 21-digit mantissa plus sign and exponent. Thus, it is to be expected that $\epsilon \approx 10^{-21}$.

While the analysis presented here is oversimplified it suggests that only about 14-place accuracy can be expected in γ_{15} for the semi-infinite interval and about 7 places in γ_{10} for the finite interval. The data in Tables II and III is, in general, no more accurate than the corresponding values of γ_n.

Independent verification of Table III by the referee to at least 12 places for $n = 1\ (1)\ 10$ indicates that the algorithm is more stable for the finite-interval case than is to be expected from this analysis.

On the other hand, a paper by Galant, which has appeared as this article was in preparation for printing, suggests that in the case of the semi-infinite interval the algorithm is less stable than is indicated by the above analysis.

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2. W. Gautschi "Recursive computation of certain integrals," *J. Assoc. Comput. Mach.*, v. 8, 1961, pp. 21–40. MR **22** #10156.

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