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**A METHOD FOR THE CALCULATION OF ABSCISSAS
AND WEIGHT FACTORS USING GAUSSIAN
INTEGRATION FOR INTEGRANDS WITH A
LOGARITHMIC SINGULARITY**

B. STEPHEN A. WILKERSON

RESEARCH AND TECHNOLOGY DEPARTMENT

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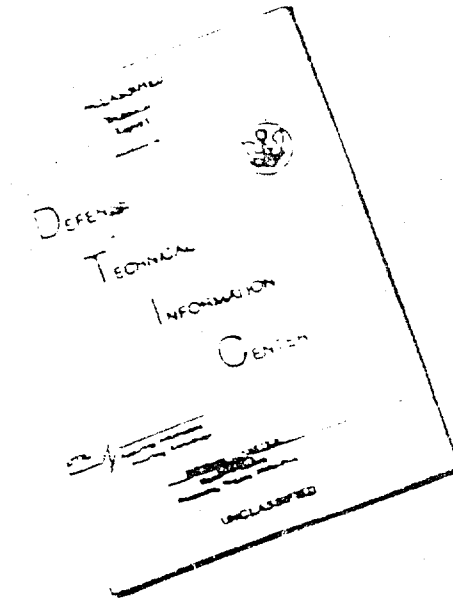


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A method for the calculation of abscissas and weight factors using Gaussian integration for integrands with a logarithmic singularity is presented. The method shows good convergent properties and allows for the accurate estimation of the error. A program is supplied for the generation of orthogonal polynomials with weight Log(x) to order n, and numerical tables for the Gaussian integration method are provided.				
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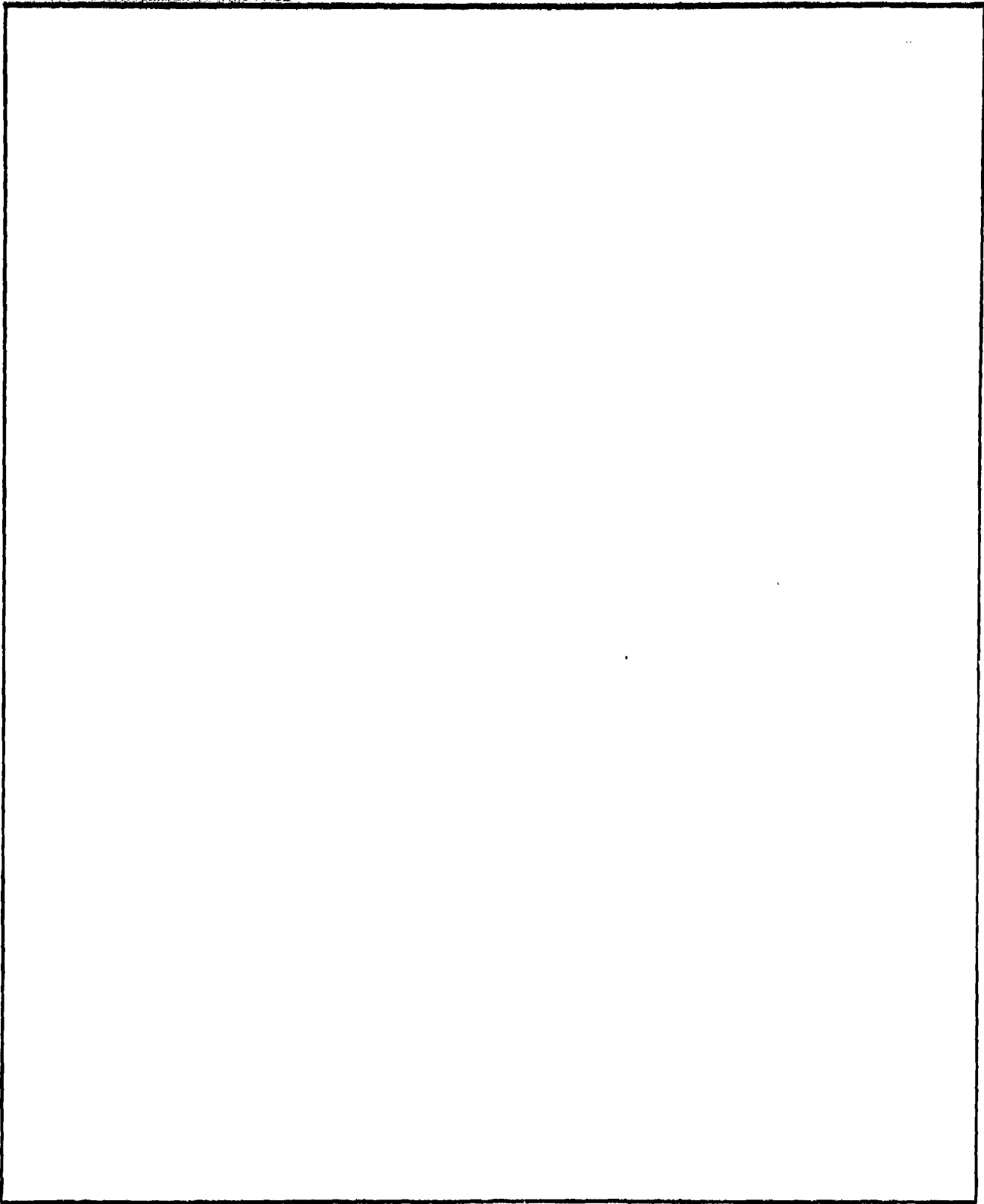
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FOREWORD

This work was sponsored under the auspices of the Naval Surface Warfare Center's long term study program. This program allows employees the opportunity of continued academic study for the period of 1 year. This study was conducted during the summer of 1987 under the aforementioned program. The purpose of this study was to approximate logarithmic singularities found in integrals by use of a Gaussian integration formulation. The method provides a simple approach to the calculation of Gaussian integration weight factors and roots. A short program is also supplied to future users on the method for similar singularities which occur in physical problems.

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Approved by:

K. F. Mueller

K. F. MUELLER, Head
Energetic Materials Division

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SECTION 1

INTRODUCTION

The expansion of a function in terms of orthogonal polynomials can be very useful. These polynomials are easy to manipulate while retaining good convergence properties. The calculation of these polynomials to higher orders is nontrivial and requires the use of a computer in order to obtain reasonable accuracy. These polynomials can then be used to construct a Gaussian integration scheme retaining a degree of precision $2m-1$ where m is the degree of the orthogonal polynomials used. The resulting error in the Gaussian method can be estimated and therefore controlled. These computations extend previous Tables which were compiled by hand calculation.^{1,2}

SECTION 2

MATHEMATICAL FORMULATION

2.1 ORTHOGONAL POLYNOMIALS

For every weight distribution there is an associated set of orthogonal polynomials.³ The polynomials are unique and independent of the choice of constants $a_0, a_1, a_2, \dots, a_n$ which can be given arbitrary nonzero values. For $n > 0$ the orthogonal polynomials will satisfy a three-term recursion relationship as follows:

$$\phi_{n+1}(x) = \alpha_n(x - \beta_n)\phi_n(x) - \gamma_n\phi_{n-1}(x)$$

with

$$\phi_{-1}(x) = 0, \quad \phi_0(x) = a_0, \quad \alpha_n = a_{n+1}/a_n$$

and

$$\beta_n = \frac{\int x \phi_n(x) \phi_n(x) dx}{\int (\phi_n(x))^2 dx} \quad (1)$$

$$\gamma_n = \frac{\int \alpha_n \phi_n(x) \times \phi_{n-1}(x) dx}{\int \phi_{n-1}(x)^2 dx}$$

In general the integrations above can become quite cumbersome and difficult to carry out by hand. However, in the case with weight $\ln(x)$, a relationship can be developed reducing the integration to a constant, dependent only on the power of x . These relationships are:

$$\int_0^1 x^n \ln(x) dx = \frac{(-1)}{(n+1)^2} \quad (2)$$

$$\int_{-1}^1 x^n \ln(x) dx = \frac{(1+(-1)^n)}{(n+1)^2} \quad (3)$$

Making use of these relationships, the problem can be broken-down into the manipulation of polynomials in addition, subtraction and multiplication. This type of calculation is well suited for computer programming. For simplicity we will set the $a_0, a_1, a_2, a_3, \dots, a_n$ coefficients equal to one. The program can be further simplified through modulation. The final program can calculate orthogonal polynomials, with weight $\ln(x)$, to degree n .

The numerical accuracy of the polynomials is determined by the significant figures retained by the computer. Initially, it is important to retain a high degree of accuracy so that the resulting Gaussian integration scheme will retain accuracy to a significant number of decimal places. This will become more evident as the formulation for the weight factors in the Gaussian integration scheme are developed. For now a 34 decimal place accuracy, which is the limit of VAX FORTRAN Quad precision, is retained. The first four orthogonal polynomials for weight $\ln(x)$ in the interval $0 \leq x \leq 1$ are:

$$\begin{aligned} \phi_0 &= 1 \\ \phi_1 &= x - (1/4) \\ \phi_2 &= x^2 - (5/7)x + (17/252) \\ \phi_3 &= x^3 - (3105/2588)x^2 + (178281/501425)x - (4679/258800) \end{aligned}$$

These polynomials are given in decimal form to order ϕ_8 in Appendix A. Using the same nomenclature, the orthogonal polynomials for $\ln[1/|x|]$ in the interval $-1 \leq x \leq 1$ are:

$$\begin{aligned} \phi_0 &= 1 \\ \phi_1 &= x \\ \phi_2 &= x^2 - (1/9) \\ \phi_3 &= x^3 - (9/25)x \end{aligned}$$

These polynomials are also given to order ϕ_8 in Appendix B. From the recursion relationship for ϕ_n , each new polynomial is observed to depend on the accuracy of the previous polynomial. For operations in addition, this will result in the loss of significant figures roughly equivalent to their deviation from unity. This is a factor in the computation over the interval

$0 \leq x \leq 1$ which has higher variations in the polynomial's constants than for the interval $-1 \leq x \leq 1$. Therefore, care was taken in the calculation of the corresponding roots and the weights used in the Gaussian integration scheme to control the roundoff error. The roots of the polynomials were calculated using a standard Newton-Raphson method. The method allowed the accuracy of the roots to be controlled to a specified number of significant figures. Twenty-four decimal places were retained allowing 10 decimal places to be lost in the original computation of the orthogonal polynomials. A higher accuracy in the calculation of the orthogonal polynomials would result in more significant digits in the Gaussian integration scheme, which could be accomplished with some clever programming techniques. However, it was felt for general applications a 16 to 20 decimal place accuracy in the final Gaussian integration would be sufficient. The computer program used in the calculations is provided in Appendix C. The program is capable of calculating orthogonal polynomials weight $w(x)$ to order n within the limitations of the computer used.

2.2 GAUSSIAN QUADRATURE

The Gaussian quadrature formulation will be discussed to show how weight and error factors in the Gaussian integration scheme are calculated. The description of the method will show the link between the orthogonal polynomials calculated in Section 2.1 and the resulting Gaussian quadrature formulation. The basic formula for Gaussian integration is:

$$\int_a^b f(x)w(x)dx = \sum_{j=1}^m H_j f(x_j) + \frac{f^{(2m)}(\xi)}{(2m)!} \int_a^b [\pi(x)]^2 w(x) dx \quad (4)$$

where, H_j is the Gaussian integration weight factor and x_j terms are the roots of the orthogonal polynomials, of order m , which were calculated in Section 2.1. The error is a function of the $2m^{\text{th}}$ derivative of $f(x)$ and $\pi(x)$ will be given in the Gaussian Quadrature development. The formulation follows the nomenclature given in F. B. Hildebrand's classic book, "Introduction to Numerical Analysis."⁴

The formulation begins by noting that the values of $f(x)$ and its derivative $f'(x)$ are known at m points between a and b in ascending order, $a < x_1 < x_2 < x_3 < \dots < x_m < b$. The

auxiliary functions:

$$\pi(x) = (x - x_1)(x - x_2)\dots(x - x_m) \quad (5)$$

and

$$l_i(x) = \frac{\pi(x)}{(x - x_i)\pi'(x_i)} \quad (i=1, 2, \dots, m) \quad (6)$$

can now be constructed which have the following properties, $\pi(x_i) = 0$, with $l_i(x_i) = \delta_{ij}$. These important relationships are used to assemble a polynomial of order $m-1$ which takes on the values of $f(x_1), f(x_2), \dots, f(x_m)$ in the interval a to b . The resulting expression is written as:

$$y(x) = \sum_{k=1}^m l_k(x) f(x_k) \quad (7)$$

The error in the expression has the form:

$$E = \frac{f^{(m)}(\xi)}{m!} \pi(x) \quad (8)$$

where ξ is in the interval $a < \xi < b$. Now, taking advantage of the fact that $f(x)$ and $f'(x)$ are known, a polynomial of degree $2m-1$ with $2m$ parameters can be written as:

$$y(x) = \sum_{k=1}^m h_k(x) f(x_k) + \sum_{k=1}^m \underline{h}_k(x) f'(x_k) \quad (9)$$

where $h_i(x)$ and $\underline{h}_i(x)$ are polynomials of order $2m-1$. To satisfy for $y(x_j) = f(x_j)$, the following must hold for $h_i(x_j) = \delta_{ij}$ and $\underline{h}_i(x_j) = 0$. Similarly, for $y'(x_j) = f'(x_j)$, then the values $h_i(x_j) = 0$, and $\underline{h}_i(x_j) = \delta_{ij}$ must hold. Making use of the auxiliary function $l_i(x)$, which is degree $m-1$, $h_i(x)$ and $\underline{h}_i(x)$ can be written as:

$$h_i(x) = r_i(x) [l_i(x)]^2 \quad (10)$$

and

$$\underline{h}_i(x) = s_i(x) [l_i(x)]^2 \quad (11)$$

These relationships have order $2m-1$ and $r_i(x_i)$ and $s_i(x_i)$ are linear functions satisfying $r_i(x_i) = 1$, $r'_i(x_i) + 2l'_i(x_i) = 0$, $s_i(x_i) = 0$ and $s'_i(x_i) = 1$. Combining these expressions yields:

$$h_i(x) = [1 - 2l'_i(x_i)(x - x_i)][l_i(x)]^2 \quad (12)$$

and

$$h_i(x) = (x - x_i)[l_i(x)]^2 \quad (13)$$

which with Equation (9) is known as Hermite's interpolation formula. The error associated with Equation (9) is given by:

$$E = \frac{f^{(2m)}(\xi)}{(2m)!} [\pi(x)]^2 \quad (14)$$

Now taking $y(x)$ as $f(x)$ the integral is written as:

$$\begin{aligned} \int_a^b f(x)w(x)dx &= \\ \sum_{j=1}^m f(x_j) \int_a^b w(x)[1 - 2l'_k(x_k)(x-x_k)][l_k(x)]^2 dx &+ \\ \sum_{j=1}^m f'(x_j) \int_a^b w(x)(x-x_k)[l_k(x)]^2 dx &+ \\ \frac{f^{(2m)}(\xi)}{(2m)!} \int_a^b w(x)[\pi(x)]^2 & \end{aligned} \quad (15)$$

If $\pi(x)$ is orthogonal to $l_1(x), l_2(x), \dots, l_m(x)$ over (a, b) relative to the weighting functions $w(x)$, the second term in Equation (15) will vanish and the resulting expression will reduce to:

$$\int_a^b f(x)w(x)dx = \sum_{j=1}^m H_j f(x_j) + \frac{f^{(2m)}(\xi)}{(2m)!} \int_a^b [\pi(x)]^2 w(x) dx \quad (16)$$

with

$$H_k = \int_a^b w(x)[l_k(x)]^2 dx \quad (17)$$

while retaining accuracy of $2m-1$. Rather than calculating the Gaussian Integration weight factors H_j directly from Equation (17), which could become quite difficult, they can be determined by taking advantage of Equation (16)'s $2m-1$ accuracy and allowing $f(x) = x^m$. With $m = 0, 1, 2 \dots m-1$ Equation (16) can be calculated exactly. The result will yield a matrix:

$$A_{ij} H_j = \int_a^b x^i \ln(1/|x|) dx = \text{const.} \quad (i=0,1,\dots,m-1) \quad (18)$$

where

$$A_{ij} = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ x_1 & x_2 & x_3 & \dots & x_m \\ x_1^2 & x_2^2 & x_3^2 & \dots & x_m^2 \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & x_m^{m-1} \end{bmatrix}$$

Equation (18) can be solved yielding the values of the weight H_j using a Gaussian elimination routine. The drawback in this method is the loss in accuracy from the Gaussian elimination. When increased accuracy is required, the Gaussian weight factors can be calculated directly using Equation (17). However, for most applications the above method is sufficient.

SECTION 3

RESULTS

The results from Equation (16) are tabulated in Tables 1 and 2. The numerical accuracy was verified through the calculation of a polynomial of order $2m-1$. The Gaussian quadrature should, in this case, be exact. Comparing the Gaussian solution to the exact solution gave an estimation of the total number of significant figures accuracy. As expected, the accuracy was higher for the lower order polynomials than for the higher order polynomials. Further, the accuracy was roughly 16 decimal places in the worst case. Therefore, only the first 16 decimal places are given. All of the polynomials were checked using this procedure.

TABLE 1. GAUSSIAN QUADRATURE $\ln(x)$ $0 \leq x \leq 1$

$$\int_0^1 f(x) \text{Log}(1/|x|) dx = \sum_{j=1}^m \alpha_j f(x_j) + \frac{f^{(2m)}(\xi)}{(2m)!} K_m$$

x_j				α_j		
			n=2			
0.11200	88061	66976		0.71853	93190	30384
0.60227	69081	18738		0.28146	06809	69616
			n=3			
0.06389	07930	87325		0.51340	45522	32363
0.36899	70637	15618		0.39198	00412	01488
0.76688	03039	38941		0.09461	54065	66149
			n=4			
0.04144	84001	99383		0.38346	40681	45135
0.24527	49143	20602		0.38687	53177	74763
0.55616	54535	60276		0.19043	51269	50142
0.84898	23945	32985		0.03922	54871	29960
			n=5			
0.02913	44721	51972		0.29789	34717	82894
0.17397	72133	20898		0.34977	62265	13224
0.41170	25202	84902		0.23448	82900	44052
0.67731	41745	82820		0.09893	04595	16633
0.89477	13610	31008		0.01891	15521	43196
			n=6			
0.02163	40058	44117		0.23876	36625	78548
0.12958	33911	54951		0.30828	65732	73947
0.31402	04499	14766		0.24531	74265	63210
0.53865	72173	51802		0.14200	87565	66477
0.75691	53373	77403		0.05545	46223	24886
0.92266	88513	72120		0.01016	89586	92932
			n=7			
0.01671	93554	08259		0.19616	93894	25248
0.10018	56779	15675		0.27030	26442	47273
0.24629	42462	07931		0.23968	18730	07691
0.43346	34932	57033		0.16577	57748	10433
0.63235	09880	47766		0.08894	32271	37658
0.81111	86267	40106		0.03319	43043	56571
0.94084	81667	43348		0.00593	27870	15126

TABLE 1. (Cont.)

x_i				α_i		
			n=8			
0.01332	02441	60892		0.16441	66047	28003
0.07975	04290	13895		0.23752	56100	23306
0.19787	10293	26188		0.22684	19844	31919
0.35415	39943	51909		0.17575	40790	06070
0.52945	85752	34917		0.11292	40302	46759
0.70181	45299	39100		0.05787	22107	17782
0.84937	93204	41107		0.02097	90737	42133
0.95332	64500	56360		0.00368	64071	04028
			n=9			
0.01086	93360	84175		0.14006	84387	48135
0.06498	36663	38008		0.20977	22052	01030
0.16222	93980	23883		0.21142	71498	96603
0.29374	99039	71675		0.17715	62339	38080
0.44663	18819	05468		0.12779	92280	33205
0.60548	16627	76129		0.07847	89026	11562
0.75411	01371	57164		0.03902	25049	85399
0.87726	58288	35838		0.01386	72955	49593
0.96225	05594	10282		0.00240	80410	36392
			n=10			
0.00904	26309	62200		0.12095	51319	54571
0.05397	12662	22501		0.18636	35425	64072
0.13531	18246	39251		0.19566	08732	77760
0.24705	24162	87160		0.17357	71421	82907
0.38021	25396	09332		0.13569	56729	95484
0.52379	23179	71843		0.09364	67585	38111
0.66577	52055	16425		0.05578	77273	51416
0.79419	04160	11966		0.02715	98108	99233
0.89816	10912	19004		0.00951	51826	02849
0.96884	79887	18634		0.00163	81576	33598
			n=11			
0.00764	39411	74638		0.10565	22560	99100
0.04554	18282	56579		0.16657	16806	00629
0.11452	22974	55125		0.18056	32182	87754
0.21037	85812	27034		0.16727	87367	73784
0.32669	55532	21693		0.13869	70574	01631
0.45545	32469	28813		0.10393	34333	65044
0.58764	83563	59084		0.06953	66978	88735
0.71396	38500	12561		0.04054	16008	03596
0.82545	32178	01812		0.01943	54024	76218
0.91419	39216	12543		0.00673	74293	42450
0.97386	02562	75586		0.00115	24869	61057

TABLE 1. (Cont.)

x_i		a_i
	n=12	
0.00654	87222 79080	0.09319 26914 43931
0.03894	68095 60450	0.14975 18275 76322
0.09815	02631 06007	0.16655 74543 64593
0.18113	85815 90632	0.15963 35594 36988
0.28322	00676 67373	0.13842 48318 64836
0.39843	44351 63437	0.11001 65706 35721
0.51995	26267 92353	0.07996 18217 70829
0.64051	09167 16106	0.05240 69548 24642
0.75286	50120 51831	0.03007 10888 73761
0.85024	00241 62302	0.01424 92455 87998
0.92674	96832 23914	0.00489 99245 82322
0.97775	61296 89997	0.00083 40290 38057
	n=16	
0.00389	78344 87115	0.06079 17100 43591
0.02302	89456 16873	0.10291 56775 17581
0.05828	03983 06240	0.12235 56620 46009
0.10867	83650 91053	0.12756 92469 37015
0.17260	94549 09843	0.12301 35746 00070
0.24793	70544 70578	0.11184 72448 55485
0.33209	45491 29916	0.09659 63851 52124
0.42218	39105 81948	0.07935 66643 51473
0.51508	24733 81462	0.06185 04945 81965
0.60755	61204 47728	0.04543 52465 07726
0.69637	56532 28213	0.03109 89747 51581
0.77843	25658 73265	0.01945 97659 27360
0.85085	02697 15391	0.01077 62549 63205
0.91108	68572 22271	0.00497 25428 90087
0.95702	55717 03542	0.00167 82011 10051
0.98704	78002 47984	0.00028 23537 64668
	n=20	
0.00258	83279 57950	0.04314 27521 61381
0.01520	96623 61051	0.07538 37099 48624
0.03853	65503 98586	0.09305 32674 85084
0.07218	16138 58240	0.10145 67118 65901
0.11546	05265 41834	0.10320 17620 51262
0.16744	28563 32738	0.10002 25497 82060
0.22698	37873 09246	0.09325 97992 65015
0.29275	49609 69755	0.08402 89528 32386
0.36327	74298 53964	0.07328 55890 93483
0.43695	71400 46558	0.06185 03368 85688
0.51212	25945 90821	0.05041 66044 21955

TABLE 1. (Cont.)

x_1			α_1		
n=20 (cont.)					
0.58706	40447	84407	0.03955	13700	01102
0.66007	34131	51321	0.02969	40779	02129
0.72948	40837	46511	0.02115	63153	68784
0.79370	96718	02302	0.01412	37329	58045
0.85128	08926	21665	0.00866	09745	19127
0.90087	96807	20293	0.00471	99401	57046
0.94136	97490	37632	0.00215	13974	10105
0.97182	27410	26546	0.00071	97282	17043
0.99153	80814	23101	0.00012	04276	76769

Error Factor

m	K_m
2	2.8527E-03
3	1.7324E-04
4	1.0651E-05
5	6.5868E-07
6	4.0864E-08
7	2.5401E-09
8	1.5809E-10
9	9.8482E-12
10	6.1386E-13
11	3.8281E-14
12	1.4902E-16
16	3.6251E-20
20	5.5140E-25

TABLE 2. GAUSSIAN QUADRATURE $\ln(x)$ $-1 \leq x \leq 1$

$$\int_{-1}^1 f(x) \text{Log}(1/|x|) dx = \sum_{j=1}^m a_j f(x_j) + \frac{f^{(2m)}(\xi)}{(2m)!} K_m$$

$\pm x_j$	a_j
	n=2
0.33333 33333 33333	1.00000 00000 00000
	n=3
0.00000 00000 00000	1.38271 60493 82716
0.60000 00000 00000	0.30864 19753 08641
	n=4
0.21304 15047 38934	0.86489 96815 02982
0.72929 60938 31051	0.13510 03184 97017
	n=5
0.00000 00000 00000	1.09457 98791 69950
0.42048 98338 89206	0.38776 70148 27492
0.80943 17212 07776	0.06494 30455 87532
	n=6
0.15842 27734 26985	0.74816 53867 89280
0.55266 10734 15253	0.21593 27476 27900
0.85720 27159 35678	0.03590 18655 82819
	n=7
0.00000 00000 00000	0.91905 14893 96716
0.32384 19262 08046	0.39366 19293 55519
0.65016 59292 67686	0.12579 98534 11872
0.89012 86734 99548	0.02101 24725 34250
	n=8
0.12670 24568 20194	0.65995 61516 92837
0.44261 10087 71680	0.24698 40796 71079
0.71755 21511 92643	0.07977 87676 46011
0.91233 97218 17349	0.01328 10009 90071
	n=9
0.00000 00000 00000	0.79842 97904 94917
0.26359 77526 12729	0.38007 36092 67535
0.53829 17961 34696	0.15972 57440 76797
0.76891 63270 11850	0.05227 98022 93951
0.92882 94062 74082	0.00870 59491 14257
	n=10
0.10583 33779 87174	0.59201 93756 79453
0.36867 78218 46622	0.25603 33044 69505
0.61013 09472 43461	0.10991 55004 92604
0.80678 01136 00994	0.03604 02553 78796
0.94084 47632 28488	0.00599 15639 79640

TABLE 2. (Cont.)

$\pm x_i$				α_i		
			n=11			
0.00000	00000	00000		0.70942	89331	43886
0.22243	43034	60040		0.36155	85459	06289
0.45787	79636	99688		0.17673	87580	04816
0.66836	54488	33843		0.07732	25140	30155
0.83674	53191	58890		0.02543	75641	71794
0.95022	91816	34761		0.00422	81513	15001
			n=12			
0.09100	68674	23150		0.53816	26831	93826
0.31583	07442	07888		0.25536	33595	74900
0.52845	71620	84128		0.12833	91477	72704
0.71382	37584	10345		0.05646	84502	49006
0.85989	86117	07467		0.01858	07671	94375
0.95743	35931	44926		0.00308	55920	15185
			n=16			
0.07127	02281	56883		0.45796	46784	03328
0.24549	21041	38222		0.24337	28614	54429
0.41504	86112	42911		0.14477	44109	75228
0.57258	30249	25674		0.08331	93142	30436
0.71203	16306	51971		0.04368	02453	94013
0.82823	11539	92066		0.01942	70191	64386
0.91694	65068	45198		0.00639	99817	92819
0.97496	24353	08112		0.00106	14885	85358
			n=20			
0.05868	47133	89643		0.40077	93096	05514
0.20085	59097	43386		0.22788	83640	17951
0.34102	34666	56996		0.14812	36002	33447
0.47499	75568	52187		0.09654	78165	51015
0.59933	10571	29593		0.06064	97491	22039
0.71098	63017	59170		0.03560	94026	12321
0.80729	48807	41148		0.01880	39939	42658
0.88597	99593	38351		0.00837	97607	34035
0.94519	16589	77233		0.00276	04277	99584
0.98353	84534	54727		0.00045	75753	81431
			n=24			
0.04993	72373	84857		0.35769	00293	66895
0.17001	63351	91168		0.21288	86057	68788
0.28921	06925	78442		0.14615	86826	93945
0.40487	40752	50707		0.10231	58022	81275
0.51485	72812	17607		0.07069	44002	80834
0.61724	49695	71121		0.04728	27060	95115
0.71030	37964	75204		0.03005	40087	21456

TABLE 2. (Cont.)

$\pm x_1$			a_1		
n=24 (cont.)					
0.79248	06376	38201	0.01773	83730	49261
0.86241	47885	90768	0.00938	59493	37033
0.91895	35961	89744	0.00418	47379	38628
0.96116	74429	07463	0.00137	83013	39528
0.98836	05896	81911	0.00022	84031	27225
n=28					
0.04349	41764	00850	0.32390	31439	72538
0.14742	92818	32779	0.19930	42967	33486
0.25100	39598	04491	0.14203	37892	50395
0.35241	93609	10315	0.10412	77083	39644
0.45023	89711	34220	0.07627	46613	85082
0.54318	11449	52526	0.05499	11928	92602
0.63006	96133	34514	0.03856	77165	33202
0.70982	40062	92755	0.02599	72305	72777
0.78146	25013	15631	0.01659	02486	69573
0.84410	84878	12482	0.00981	00812	72568
0.89699	83042	16216	0.00519	45033	21041
0.93948	87558	94016	0.00231	62505	40379
0.97106	36416	52642	0.00076	27924	50803
0.99133	76283	29069	0.00012	63840	65902
n=34					
0.03647	71393	63964	0.28480	88700	72993
0.12297	98221	19973	0.18173	17245	19901
0.20946	47888	96709	0.13455	47332	93387
0.29481	97514	16519	0.10319	69140	06127
0.37818	01056	68895	0.07983	50423	79525
0.45877	99845	11221	0.06153	96373	69396
0.53591	10708	28227	0.04689	14786	45456
0.60891	09589	81738	0.03508	51754	12643
0.67716	09074	73224	0.02560	50459	80362
0.74008	70785	20741	0.01808	47481	86851
0.79716	31474	66867	0.01223	88747	32165
0.84791	33925	37128	0.00782	68355	03823
0.89191	58393	78835	0.00463	27525	51770
0.92880	52304	04085	0.00245	39343	26313
0.95827	56693	32595	0.00109	42328	21961
0.98008	27591	90213	0.00036	03099	08124
0.99404	42773	90478	0.00005	96902	89197

TABLE 2. (Cont.)

	<u>Error Factor</u>
	K_m
2	5.5309E-02
3	1.2016E-02
4	3.0609E-03
5	7.1423E-04
6	1.8184E-04
7	4.3511E-05
8	1.1052E-05
9	2.6774E-06
10	6.7860E-07
11	1.6560E-07
12	4.1898E-08
16	1.6110E-10
20	6.2325E-13
24	2.4186E-15
28	9.4030E-18
34	2.2840E-21

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APPENDIX A

ORTHOGONAL POLYNOMIALS WEIGHT $\ln(x)$ $0 \leq x \leq 1$

$$\phi_n = \sum a_i x^i \quad a_i \quad (i=0,n)$$

n	a_0	a_1	a_2
0	1.00000000		
1	-0.25000000,	1.00000000	
2	0.06746032,	-0.71428571,	1.00000000
3	-0.01807960, 1.00000000	0.35554869,	-1.199768161,
4	0.00480026, -1.69187124,	-0.14966864, 1.00000000	0.885229712,
5	-0.00126470, 1.66127218,	0.05703065, -2.18689974,	-0.514118407, 1.00000000
6	0.00033117, -1.23444544, 1.00000000	-0.02032932, 2.68540097,	0.257587994, 2.683479253,
7	-0.00008630, 0.76866244, -3.18098055,	0.00690690, -2.43476271, 1.00000000	-0.116584253, 3.958396326,
8	0.00002240, -0.42271739, 5.48066379,	-0.0022629, 1.8144789, -3.6790746,	0.048965172, -4.239611389, 1.00000000

APPENDIX B

ORTHOGONAL POLYNOMIALS WEIGHT $\ln(x)$ $-1 \leq x \leq 1$

$$\phi_n = \sum a_i x^i \quad a_i \quad (i=0, n)$$

n	a_0	a_1	$a_2 \dots$
0	1.00000000		
1	0.00000000,	1.00000000	
2	-0.11111111,	0.00000000,	1.00000000
3	0.00000000, 1.00000000	-0.36000000,	0.00000000,
4	2.41399417, 0.00000000,	0.00000000, 1.00000000	-0.577259475,
5	0.00000000, -0.83199141,	0.11584344, 0.00000000,	0.00000000, 1.00000000
6	-5.63274451, 0.00000000, 1.00000000	0.00000000, -1.06532853,	0.250539503, 0.00000000,
7	0.00000000, 0.46235607, 0.00000000,	-3.51253083, 0.00000000, 1.00000000	0.00000000, -1.319918384,
8	1.34782840, 0.00000000, -1.55920288,	0.00000000, 0.71727267, 0.00000000,	-9.507552587, 0.00000000, 1.00000000

APPENDIX C
COMPUTER PROGRAM

Due to the relative simplicity of the programs, only a few comment cards are included. However, a brief explanation of the program's structure and subroutines will allow modification or improvement for the calculation of a variety of orthogonal polynomials. The programs make use of the recursion relationship in Equation (1) and the integral evaluations given by Equations (2) and (3) of Section 2.1 respectively. POLY1 is more general and calculates both Gamma γ and Beta β from Equation (1). However, in POLY2, Beta is zero and therefore not included. Both programs have the three subroutines, POLYMULT, POLYINT, and POLYPLUS. POLYMULT multiplies two polynomials and stores the result in a third polynomial in ascending orders of x . POLYINT integrates a polynomial and returns a real expression in accordance with Equations (2) and (3). POLYPLUS multiplies a polynomial by x . The working polynomials are stored in arrays A through C and the results are stored in ANS. Each polynomial is dependent on the previous polynomial, and the program is looped "n" times to calculate all polynomials to order $n+1$.

PROGRAM POLY1

PROGRAM POLY1

C 0 < x < 1

```

PROGRAM POLY1
IMPLICIT REAL*16 (A-H,P-Z)
DIMENSION A(80),B(80),C(80)
COMMON /AAA/ANS(80,80)
ANS(1,1)=1.0Q0
ANS(2,2)=1.0Q0
ANS(2,1)=-.25Q0
DO 11 N=2,20
DO 7 I=1,N+1
A(I)=0.0Q0
B(I)=0.0Q0
7 C(I)=0.0Q0

```

C
C
C
FIND A(I)

```

DO 1 I=1,N
1 A(I)=ANS(N,I)
CALL POLYPLUS(A,N)
CALL BETA(B,N)
CALL GAMA(C,N)

```

C
C
C
CALCULATE POLY

```

DO 6 I=1,N+1
6 ANS(N+1,I)=(A(I)-B(I))-C(I)

```

```

WRITE(6,*)N+1
DO 10 I=1,N+1
10 WRITE(6,*)ANS(N+1,I)
11 CONTINUE
STOP
END

```

C
C
C
FIND BETA

```

SUBROUTINE BETA(E,N)
IMPLICIT REAL*16 (A-H,P-Z)
DIMENSION A(80),B(80),C(80),D(80),E(80)
COMMON /AAA/ANS(80,80)
DO 1 I=1,N+1
A(I)=0.0Q0
B(I)=0.0Q0

```

PROGRAM POLY1 (Cont.)

```

C(I)=0.0Q0
1 D(I)=0.0Q0
  DO 2 I=1,N
    A(I)=ANS(N,I)
    B(I)=A(I)
2 C(I)=A(I)
  CALL POLYPLUS(A,N)
  CALL POLYMULT(D,P,C,N,N)
  CALL POLYINT(D,DD,2*N)
  CALL POLYMULT(D,A,B,N+1,N)
  CALL POLYINT(D,DD1,2*N+1)
  DO 3 I=1,N
3 E(I)=(DD1/DD)*B(I)
  RETURN
  END

```

C
C
C

FIND GAMA

```

SUBROUTINE GAMA(D,N)
  IMPLICIT REAL*16 (A-H,P-Z)
  DIMENSION A(80),B(80),C(80),D(80)
  COMMON /AAA/ANS(80,80)
  DO 1 I=1,N+1
    A(I)=0.0Q0
    B(I)=0.0Q0
    C(I)=0.0Q0
1 D(I)=0.0Q0
  DO 2 I=1,N
2 A(I)=ANS(N,I)
  CALL POLYPLUS(A,N)
  DO 3 I=1,N-1
3 B(I)=ANS(N-1,I)
  CALL POLYMULT(C,A,B,N+1,N-1)
  CALL POLYINT(C,CC,2*N)
  DO 4 I=1,N+1
4 A(I)=B(I)
  CALL POLYMULT(C,B,A,N-1,N-1)
  CALL POLYINT(C,CC1,2*(N-1))
  XNUMB=CC/CC1
  DO 5 I=1,N-1
5 D(I)=ANS(N-1,I)*XNUMB
  RETURN
  END
SUBROUTINE POLYMULT(A,B,C,K,L)
  IMPLICIT REAL*16 (A-H,P-Z)
  DIMENSION A(80),B(80),C(80)
  DO 1 I=1,K+L
1 A(I)=0.0Q0
  DO 2 I=1,K

```

PROGRAM POLY1 (Cont.)

```

DO 2 J= 1,L
2 A(I+J-1)=A(I+J-1)+B(I)*C(J)
RETURN
END

```

C
C
C

INTEGRATION ROUTINE

```

SUBROUTINE POLYINT(A,AA,N)
IMPLICIT REAL*16 (A-H,P-Z)
DIMENSION A(80)
AA=0.0Q0
DO 1 I=1,N-1
1 AA=AA+A(I)*(-1.0Q0)/(QFLOAT(I)**2)
RETURN
END

```

C
C
C

SHIFTS THE POLY BY ONE

```

SUBROUTINE POLYPLUS(A,N)
IMPLICIT REAL*16 (A-H,P-Z)
DIMENSION A(80),B(80)
DO 1 I=1,N+1
1 B(I+1)=A(I)
DO 2 I=1,N+1
2 A(I)=B(I)
RETURN
END

```

PROGRAM POLY2

PROGRAM POLY2

```

C      -1 < x < 1

      IMPLICIT REAL*16 (A-H,P-Z)
      DIMENSION A(80),B(80),C(80)
      COMMON /AAA/ANS(80,80)
      ANS(1,1)=1.0Q0
      ANS(2,2)=1.0Q0
      DO 11 N=2,36
      DO 7 I=1,N+1
      A(I)=0.0Q0
      B(I)=0.0Q0
7     C(I)=0.0Q0

      FIND A(I)

      DO 1 I=1,N
1     A(I)=ANS(N,I)
      CALL POLYPLUS(A,N)
      CALL GAMA(C,N)

      CALCULATE POLY

      DO 6 I=1,N+1
6     ANS(N+1,I)=A(I)-C(I)

      WRITE(6,*)N+1
      DO 10 I=1,N+1
10    WRITE(6,*)ANS(N+1,I)
11    CONTINUE
      STOP
      END

      FIND GAMA

      SUBROUTINE GAMA(D,N)
      IMPLICIT REAL*16 (A-H,P-Z)
      DIMENSION A(80),B(80),C(80),D(80)
      COMMON /AAA/ANS(80,80)
      DO 1 I=1,N+1
      A(I)=0.0Q0
      B(I)=0.0Q0
      C(I)=0.0Q0
1     D(I)=0.0Q0
      DO 2 I=1,N

```

PROGRAM POLY2 (Cont.)

```

2 A(I)=ANS(N,I)
  CALL POLYPLUS(A,N)
  DO 3 I=1,N-1
3 B(I)=ANS(N-1,I)
  CALL POLYMULT(C,A,B,N+1,N-1)
  CALL POLYINT(C,CC,2*N)
  DO 4 I=1,N+1
4 A(I)=B(I)
  CALL POLYMULT(C,B,A,N-1,N-1)
  CALL POLYINT(C,CC1,2*(N-1))
  XNUMB=CC/CC1
  DO 5 I=1,N-1
5 D(I)=ANS(N-1,I)*XNUMB
  RETURN
  END
  SUBROUTINE POLYMULT(A,B,C,K,L)
  IMPLICIT REAL*16 (A-H,P-Z)
  DIMENSION A(80),B(80),C(80)
  DO 1 I=1,K+L
1 A(I)=0.0Q0
  DO 2 I=1,K
  DO 2 J= 1,L
2 A(I+J-1)=A(I+J-1)+B(I)*C(J)
  RETURN
  END

```

C
C
C

INTEGRATION ROUTINE

```

SUBROUTINE POLYINT(A,AA,N)
  IMPLICIT REAL*16 (A-H,P-Z)
  DIMENSION A(80)
  AA=0.0Q0
  DO 1 I=1,N-1
1 AA=AA+A(I)*(-(1.0Q0+(-1.0Q0)**(I-1))/(QFLOAT(I)**2))
  RETURN
  END

```

C
C
C

SHIFTS THE POLY BY ONE

```

SUBROUTINE POLYPLUS(A,N)
  IMPLICIT REAL*16 (A-H,P-Z)
  DIMENSION A(80),B(80)
  DO 1 I=1,N+1
1 B(I+1)=A(I)
  DO 2 I=1,N+1
2 A(I)=B(I)
  RETURN
  END

```

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