Evaluation of an Integral Arising in Numerical Integration Near a Logarithmic Singularity

This paper is concerned with the evaluation of

$$(1) \quad I = \int_0^y x^{-1} dx \int_0^x f(u) du$$

in terms of values of f . If this integral is known, the evaluation of

$$(2) \quad I_1 = \int_0^y f(x) \log x dx$$

is readily accomplished. For, let

$$(3) \quad I_2 = \log y \int_0^y f(x) dx.$$

If f is bounded, then

$$(4) \quad I = - \int_0^y f(x) \log \frac{x}{y} dx = -I_1 + I_2;$$

the two forms for I converge or diverge together. Equation (4) follows from (2) by partial integration. Now the integral in (3) can be approximated by any one of several standard methods. The approximate evaluation of (2) can therefore be achieved, once the evaluation of (1) is completed. In this note coefficients of the Lagrangian type are presented to facilitate the computation of I . A rigorous treatment of the error is also presented.

Let

$$(5) \quad \int_0^{rh} x^{-1} dx \int_0^x f(u) du = (rh/D_n) \sum_{j=0}^n \gamma_{jr}^{(n)} f_j + R_{nr},$$

where the coefficients $\gamma_{jr}^{(n)}/D_n$ are such that the remainder R_{nr} vanishes whenever $f(u)$ is a polynomial in u of degree n ,

$$D_n = \sum_{j=0}^n \gamma_{jr}^{(n)},$$

and D_n is independent of r , and f_j are the tabular values of $f(u)$ at the points $u = jh$, $j = 0(1)n$. Thus, we assume that $f(u)$ may be adequately represented by the $(n+1)$ point Lagrangian polynomial. The interpolating polynomials are easily derived and have recently been published for $n = 1(1)10$ by SALZER [1]. The coefficients $\gamma_{jr}^{(n)}$ and D_n are then readily evaluated in a straightforward manner. These are given exactly in Table 1 for $n = 1(1)10$, $r = 1(1)(n+1)$. It is understood that $\gamma_{jr}^{(n)} = 0$ if $j > n$, and the n superscript is omitted where no confusion will result. We note some properties of the integrating coefficients useful as a check on the computation.

$$(6) \quad \begin{aligned} \gamma_{jr}^{(n)} &= D_n, & r &= j = 0 \\ \gamma_{jr}^{(n)} &= 0, & r &= 0, \quad j = 1, 2, \dots \end{aligned}$$

TABLE 1
Values of the Integration Coefficients $\gamma_r^{(n)}$ and D_n

$n = 1, D_1 = 4$		$n = 2, D_2 = 72$			$n = 3, D_3 = 288$				
	$r = 1$	$r = 2$	$r = 1$	$r = 2$	$r = 3$	$r = 1$	$r = 2$	$r = 3$	$r = 4$
$\gamma_{0r}^{(n)}$	3	2	49	34	27	185	128	99	80
$\gamma_{1r}^{(n)}$	1	2	28	40	36	145	184	171	160
$-\gamma_{2r}^{(n)}$			5	2	-9	53	32	-9	-16
$\gamma_{3r}^{(n)}$						11	8	9	32

$n = 4, D_4 = 43200$					$n = 5, D_5 = 86400$				
	$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$				
γ_{0r}	26647	18352	14157	11632	10075				
γ_{1r}	26162	30992	28422	25472	22250				
$-\gamma_{2r}$	14568	9888	2808	-192	-3000				
γ_{3r}	6062	4592	4122	6272	5750				
$-\gamma_{4r}$	1103	848	693	368	-2125				

$n = 6, D_6 = 254\ 01600$					$n = 7$				
	$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$	$r = 6$	$r = 7$		
γ_{0r}	51667	35432	27297	22432	19175	16632	143815		
γ_{1r}	60459	68344	61929	55104	49375	45864	426584		
$-\gamma_{2r}$	45406	32496	15786	7936	4176	2176	135909		
γ_{3r}	28394	21904	18414	20864	21250	24624	25096		
$-\gamma_{4r}$	10341	8056	6471	4896	625	936	73901		
γ_{5r}	1627	1272	1017	832	975	4392	24136		

$n = 8, D_8 = 16384\ 0000$								$n = 9$							
	$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$	$r = 6$	$r = 7$	$r = 8$	$r = 9$						
γ_{0r}	14815625	10122440	7790355	6398720	5464325	4786200	4308815	398815	36815						
γ_{1r}	20021784	21860544	19616904	17378304	15555000	14105664	12652584	11359309	10159309						
$-\gamma_{2r}$	18966459	13972344	8165529	5277504	3699375	2781864	2159309	165096	125096						
γ_{3r}	15837296	12331136	10112976	10059776	9710000	9311616	8911616	8511616	8111616						
$-\gamma_{4r}$	8657349	6786984	5426919	4383744	2780625	1829304	1373901	1024136	774136						
γ_{5r}	2725176	2141376	1708776	1422336	1325400	1912896	1424136	1124136	924136						
$-\gamma_{6r}$	374473	294568	234963	196288	173125	103608	699377	499377	399377						

TABLE 1—Continued

$n = 7, D_7 = 1016 \ 06400$									
$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$	$r = 6$	$r = 7$	$r = 8$		
580 41849	395 27584	303 93459	249 50784	212 97925	186 57504	166 57599	149 69344		
886 31693	941 77408	838 43343	740 21888	661 35625	598 33728	546 53963	512 63488		
1014 99507	760 95072	487 89297	346 36032	265 44375	213 60672	175 68117	179 43552		
1060 71969	830 00704	673 30539	627 82464	584 18125	543 01824	502 26519	530 69824		
773 52181	608 24096	485 86311	400 78336	307 00625	243 72576	195 22531	240 75776		
365 34375	287 71200	229 62285	192 15360	170 48475	178 84800	178 27425	240 53760		
100 42449	79 13504	63 15579	52 93824	46 08125	38 25504	12 46119	27 76064		
12 20651	9 62176	7 67961	6 44096	5 59375	4 87296	5 77661	30 45376		
$n = 8, D_8 = 91445 \ 76000$									
$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$					
51316 20253	34848 31648	26773 66143	21968 32768	18745 77625					
87140 21626	90571 74016	80102 62206	70518 72256	62900 91250					
1 17150 48026	88827 82016	60163 01406	44819 01056	35715 91250					
1 47066 62002	1 15385 14432	93102 77862	83797 38112	76228 26250					
1 34119 27280	1 05597 32480	84359 29680	70186 95680	57195 50000					
84482 78542	66578 59072	53171 35002	44586 98752	38995 57750					
34839 12806	27464 40896	21936 66786	18411 02336	15973 28750					
8470 27846	6678 03136	5334 77826	4478 70976	3882 28750					
921 46157	726 50912	580 45167	487 37792	422 35625					
$n = 9, D_9 = 1016 \ 06400$									
$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$	$r = 6$	$r = 7$	$r = 8$	$r = 9$	
16418 73888	14651 75803	13254 90688	12198 18933						
56834 47296	51909 21526	47877 16096	43802 94186						
29669 01696	25333 57526	22239 27296	17086 54986						
69760 46592	64248 40702	59942 99392	49764 58722						
48046 34880	41375 95280	36893 38880	23572 36080						
36985 14432	35089 22242	33828 53632	22605 40062						
13887 36576	10643 77706	8588 53376	300 74166						
3422 68416	3240 54346	4480 86016	2378 10006						
373 01472	340 08107	217 50272	-1656 19323						

TABLE 1—Continued
 $n = 9, D_9 = 1\ 82891\ 52000$

	$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$
γ_{0r}	1 01052 61771	68451 91552	52551 95193	43100 55424	36767 23375
γ_{1r}	1 88498 51867	1 92345 93728	1 69163 58249	1 48562 35520	1 32320 69375
$-\gamma_{2r}$	2 91173 30512	2 22465 46816	1 56159 38160	1 19737 66144	97507 30000
γ_{3r}	4 26835 37744	3 35326 55360	2 69816 71536	2 37827 25632	2 13299 30000
$-\gamma_{4r}$	4 67291 75170	3 68029 04704	2 94135 33078	2 45722 65472	2 05655 16250
γ_{5r}	3 68018 77694	2 89991 57888	2 31759 43722	1 94522 71616	1 69255 31750
$-\gamma_{6r}$	2 02380 39352	1 59485 08288	1 27484 49384	1 07034 54080	92789 35000
γ_{7r}	73812 90152	58165 89056	46502 91000	39037 05984	33840 05000
$-\gamma_{8r}$	1 6061 00929	12655 47520	10119 24171	8499 66592	7363 58125
γ_{9r}	1579 78735	1244 71744	995 37093	836 10112	724 31875
	$r = 6$	$r = 7$	$r = 8$	$r = 9$	$r = 10$
γ_{0r}	32196 47616	28725 68797	25989 49888	23777 14419	21825 76000
γ_{1r}	1 19437 96032	1 09018 88333	1 00437 15584	93178 99395	88180 40000
$-\gamma_{2r}$	82414 09152	71468 96176	63209 88160	56465 54064	56370 40000
γ_{3r}	1 93365 06624	1 77034 37360	1 63592 43776	1 51544 86992	1 55614 40000
$-\gamma_{4r}$	1 76858 89920	1 55558 24494	1 39346 45248	1 25168 26482	1 38906 40000
γ_{5r}	1 54736 49024	1 42984 78418	1 33216 74752	1 23234 34446	1 45369 76000
$-\gamma_{6r}$	81618 86592	69825 11368	60883 51744	52617 17880	72042 40000
γ_{7r}	29921 42592	27282 89816	27693 05600	27048 64104	41470 40000
$-\gamma_{8r}$	6515 04384	5880 61495	5117 83936	2260 72377	5934 40000
γ_{9r}	641 00160	577 82809	520 31488	619 23447	3684 40000

TABLE 1—Continued
 $n = 10, D_{10} = 1327 \ 79243 \ 5200$

	$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$	$r = 6$
γ_{0r}	723 64189 52621	489 09074 27264	375 22920 40047	307 61897 44640	262 34643 79625	229 68808 36416
γ_{1r}	1468 50033 86692	1475 13314 41408	1291 10727 89484	1131 47319 19360	1006 48502 72500	907 70292 47232
$-\gamma_{2r}$	2563 92311 42337	1969 25667 65376	1417 12562 57355	1107 39264 13824	914 16855 58125	780 95130 20352
γ_{3r}	4298 83795 77144	3378 89045 29920	2714 62539 43656	2361 55179 90912	2098 59440 55000	1890 83037 45024
$-\gamma_{4r}$	5492 56107 29670	4324 62531 07584	3457 99557 29538	2895 06683 01312	2455 62908 28750	2136 24559 69920
γ_{5r}	5191 84386 73344	4088 62017 77664	3269 66120 00064	2745 57934 75584	2383 88072 88000	2146 08690 57024
$-\gamma_{6r}$	3569 30461 25802	2810 59613 09568	2248 11049 67694	1888 33632 30720	1636 22328 41250	1444 80295 53792
γ_{7r}	1735 89478 25352	1366 70403 93216	1093 36716 74520	918 48017 26464	795 72025 05000	704 22954 57792
$-\gamma_{8r}$	566 60784 65079	446 03612 76480	356 87421 01341	299 80479 39072	259 72515 76875	229 92421 58784
γ_{9r}	111 47034 92860	87 73828 81024	70 20606 30228	58 98058 73152	51 09534 47500	45 23700 44160
$-\gamma_{10r}$	10 00010 93125	7 87016 39488	6 29796 70071	5 29104 93184	4 58367 90625	4 05833 32800

	$r = 7$	$r = 8$	$r = 9$	$r = 10$	$r = 11$
γ_{0r}	204 89534 91179	185 36086 50752	169 53494 85765	156 39368 24000	145 99151 65511
γ_{1r}	828 00854 84188	762 40271 93344	707 35067 85060	660 80305 60000	613 11415 75372
$-\gamma_{2r}$	683 25621 18711	608 43409 61280	548 86014 59769	502 00918 80000	425 30410 06467
γ_{3r}	1723 64701 76520	1586 42871 33696	1470 66994 47672	1377 12076 80000	1182 38205 52104
$-\gamma_{4r}$	1896 51342 25674	1709 46357 16608	1557 01643 36022	1441 34085 60000	1114 73966 17170
γ_{5r}	1958 66221 03104	1804 52337 89824	1672 63513 79904	1574 84092 80000	1166 34640 67904
$-\gamma_{6r}$	1274 09088 96198	1139 82266 32704	1030 29554 90970	955 90821 60000	566 48027 12382
γ_{7r}	636 45130 59576	599 79920 17920	566 82732 30984	548 43532 80000	293 27148 47832
$-\gamma_{8r}$	207 08481 40305	186 68586 94656	155 33317 55007	135 84382 80000	-1 25980 22811
γ_{9r}	40 72648 73764	37 00645 39648	35 36682 46812	47 36209 60000	14 60395 29460
$-\gamma_{10r}$	3 65314 55443	3 32289 67936	3 08711 82429	2 06133 52000	-17 34709 27025

As a function of r , $\gamma_{jr}^{(n)}$ is a polynomial in r of degree n and so the $(n + 1)$ th difference must vanish. Hence

$$(7) \quad \Delta^{(n+1)}\gamma_{jr}^{(n)}(r) = 0.$$

Thus, employing tables of Lagrangian interpolating coefficients [2], the present entries are easily extrapolated.

Treatment of the error follows the discussion given by MILNE [3, 4]. Let $c = \max(nh, rh)$. We have

$$(8) \quad R_{nr} = \int_0^c G_{nr}(s) f^{(n+1)}(s) ds,$$

$$(9) \quad n!G_{nr}(s) = \int_0^{rh} x^{-1} dx \int_0^x (\overline{u-s})^n du - (rh/D_n) \sum_{j=0}^n \gamma_{jr}^{(n)} (\overline{jh-s})^n,$$

where

$$(10) \quad \left. \begin{aligned} (\overline{x-s})^n &= (x-s)^n & \text{if } x \geq s \\ &= 0 & \text{if } x \leq s. \end{aligned} \right\}$$

Thus $(0, c)$ is the open interval in which $G_{nr}(s)$ does not vanish identically. $G_{nr}(s)$ is said to be definite if it does not change sign in this interval, otherwise it is indefinite. If $G_{nr}(s)$ is definite, the mean value theorem applies and

$$(11) \quad R_{nr} = E_{nr} f^{(n+1)}(\xi); \quad E_{nr} = \int_0^c G_{nr}(s) ds, \\ 0 < \xi < c.$$

$$(12) \quad (n+1)!E_{nr} = rh^{n+2} \left\{ r^{n+1}/(n+2)^2 - \sum_{j=1}^n \gamma_{jr}^{(n)} j^{n+1}/D_n \right\}.$$

The latter is obtained by putting $f(x) = x^{n+1}/(n+1)!$ in (5). If we put $f(x)$ equal to the polynomial of degree $n+1$ which vanishes at $x = 0, h, \dots, nh$ and which takes the value h^{n+1} at $x = (n+1)h$ and use equations (5), (11), and (5) with n replaced by $n+1$, we see that

$$(13) \quad E_{nr} = (rh/D_{n+1}) h^{n+1} \gamma_{n+1,r}^{(n+1)},$$

since $R_{n+1,r} = 0$. Thus, except for the case $n = 10$, the error coefficients are available in Table 1. The elements for $n = 10$ are given in Table 2. These were obtained by calculating $\gamma_{11,r}^{(11)}$ and checked using (12). They are also interpolable, recognizing that $E_{10,r}/r^2$ is a polynomial in r of degree 10. Since $\lim_{r \rightarrow 0} E_{10,r}/r^2 = 1/44$ if h is unity, there are 12 entries, and the requirement that the eleventh difference vanish furnished a further check on the entries. The values were calculated to 7D and rounded to 5D for presentation.

The error given by (8) may also be appraised by

$$(14) \quad |R_{nr}| \leq \sup |f^{(n+1)}(s)| \int_0^c |G_{nr}(s)| ds.$$

Alternatively R_{nr} can be expressed in terms of an integral on one of the lower derivatives $f^{(n)}, f^{(n-1)}, \dots, f^{(1)}$ of f . The only essential advantage of definiteness is that it simplifies the evaluation of the integral in (14).

TABLE 2
Values of Error Coefficients for $n = 10$

r	E_{10r}/h^{12}
1	0.00666
2	0.01046
3	0.01257
4	0.01408
5	0.01524
6	0.01620
7	0.01701
8	0.01770
9	0.01834
10	0.01873
11	0.02454

Concerning the definiteness of $G_{nr}(s)$, general theorems are wanting, but in each case definiteness can be checked directly. It has been established that the function is definite for all reported values of r and n such that $r \leq n$. If $r = n + 1$, $G_{n,n+1}(s)$ is definite (indefinite) if n is even (odd). In the indefinite cases, $G_{n,n+1}(s)$ has one zero in the open interval $(0, n + 1)$. Let ζh be the vanishing point. Then the remainder can be decomposed into two parts. Thus,

$$(15) \quad R_{n,n+1} = f^{(n+1)}(\xi_1) \int_0^{\zeta h} G_{n,n+1}(s) ds + f^{(n+1)}(\xi_2) \int_{\zeta h}^{(n+1)h} G_{n,n+1}(s) ds$$

where $0 < \xi_1 < \zeta h < \xi_2 < (n + 1)h$. The values of ζ and the two integrals in (15) are recorded in Table 3 for $n = 1(2)9$, mostly to 5d. The zeros were evaluated by inverse interpolation using TAYLOR's theorem. Availability of the derivatives facilitated the calculation of the integrals.

The heuristic verification that $G_{nr}(s)$ is definite is straightforward, but the numerical work is considerably simplified, especially for n large, using some results due to BARRETT [5]. Let $G_{nr}^{(k)}(s)$ denote the k -th derivative of $G_{nr}(s)$ with respect to s . He has shown that $G_{nr}^{(k)}(s)$ is defined and continuous in $(0, c)$ closed for $0 \leq k \leq n - 1$. With this restriction on k , $G_{nr}^{(k)}(0) = G_{nr}^{(k)}(c) = 0$. If $\nu(k)$ denotes the number of zeros of $G_{nr}^{(k)}(s)$ in $(0, c)$ closed, then $\nu(k) \geq k + 2$ and $G_{nr}(s)$ is definite if equality holds. If $k = 0$, the condition is both necessary and sufficient. For the problem at hand, we first examined the function $G_{nr}^{(n-1)}(s)$ for $n \geq 5$. If $\nu(n - 1) = n + 1$, then $G_{nr}(s)$ is definite. In a few cases, it was found that $\nu(n - 1) = n + 2$, and in some of these definiteness was established by showing that $\nu(n - 2) = n$. In the remaining cases, $\nu(n - 2) = n + 1$, and these were

TABLE 3
Values of Zeros of $G_{n,n+1}(s)$ and Error Coefficients for the Indefinite Cases

n	ζ	$\int_0^{\zeta h} G_{n,n+1}(s) ds / h^{n+2}$	$\int_{\zeta h}^{(n+1)h} G_{n,n+1}(s) ds / h^{n+2}$
1	0.84829	-0.08602	0.03046
3	2.02495	-0.03961	0.00554
5	3.22618	-0.02661	0.00214
7	4.46830	-0.02001	0.00098
9	5.71960	-0.01602	0.00050

shown to be indefinite by examining $G_{nr}(s)$ itself. From the computational point of view, examination of the higher derivatives facilitates the study as the inconvenience of handling large powers of s is removed.

KAPLAN [6] has given coefficients to facilitate the evaluation of

$$(16) \quad \int_{r_1 h}^{r_2 h} g(x) dx$$

$$g(x) = x^\eta [A(x) \log x + B(x)], \quad \eta = 0, 1$$

in terms of values of $g(x)$. He writes

$$(17) \quad \int_{r_1 h}^{r_2 h} g(x) dx \sim h \sum_{i=\rho}^{\rho+P} c_i g(ih)$$

where ρ and $\rho + P$ are number of tabular intervals h from the singularity to the first and last of group of $P + 1$ consecutive ordinates. All formulas are derived on the basis that $A(x)$ and $B(x)$ can be represented by quadratic polynomials. For the most part, the tables can be described as follows. Coefficients c_i are given for $\rho = 1, 5, 10$ or 15 and $(r_1, r_2) = (\rho + s, \rho + s + 1)$, $s = 0(1)4$; also for $\rho = 1$ and $(r_1, r_2) = (0, 1)$, $(0, 5)$ and $(0, 6)$. Here $P = 5$. If $\eta = 0$, additional entries are presented for $\rho = 1$, $P = 4$ and $(r_1, r_2) = (s, s + 1)$, $s = 0(1)4$. The latter group are five term formulas and it is assumed that the constant term in the representation for $A(x)$ is missing. Thus, tabular values at the origin are never used. All entries are to 10D. The error term is not considered.

The principal application of Kaplan's table occurs when $A(x)$ and $B(x)$ are not individually known, but $g(x)$ only is tabulated. If each is known, then tables in present paper are more advantageous since representation of $f(x)$ by higher order polynomials is possible. Present tables are useful to integrate out to ten tabular intervals h from the singularity after which ordinary integration formulas may be employed. For integration beyond $10h$, recourse to Kaplan tables may still be appropriate depending on the nature of $f(x)$.

The problem treated in this note is an example of approximate product integration, and has been studied by BEARD [7]. Other examples have been given by SHELDON [8] and LUKE [9, 10].

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1. H. E. SALZER, "Tables of coefficients for the numerical calculation of Laplace transforms," U. S. Dept. of Commerce, AMS. 30, 1953.

2. "Tables of Lagrangian interpolation coefficients," National Bureau of Standards, Columbia University Press, 1948.

3. W. E. MILNE, "The remainder in linear methods of approximation," NBS, *Jn. of Research*, v. 43, 1949, p. 501-511.

4. W. E. MILNE, *Numerical Calculus*, Princeton University Press, p. 108-116.

5. W. BARRETT, "On the remainders of numerical formulae, with special reference to differentiation formulae," *London Math. Soc., Jn.*, v. 27, Part 4, 1952, p. 456-464. See also, "On the remainder term in numerical integration formulae," same author and journal, p. 465-470.

6. E. L. KAPLAN, "Numerical integration near a singularity," *J. Math. Phys.*, v. 26, 1952, p. 1-28.

7. R. E. BEARD, "Some notes on approximate product integration," *Inst. of Actuaries, Jn.*, v. 73, 1948, p. 356-414.

8. J. W. SHELDON, "Numerical evaluation of integrals of the form $\int_a^b f(x)g(x)dx$," *International Business Machines Corporation Seminar*, New York, 1950, p. 74-78.

9. Y. L. LUKE, "Mechanical quadrature near a singularity," *MTAC*, v. 6, 1952, p. 215-219.

10. Y. L. LUKE, "On the computation of oscillatory integrals," *Cambridge Philos. Soc., Proc.*, v. 50, 1954, p. 269-277.