Tables for Use in Quadrature Formulas Involving Derivatives of the Integrand

By George Struble

1. Introduction. Tables of the a_j and x_j in the approximate quadrature formulas developed by Hammer and Wicke [1]

$$(1)\qquad \int_{-1}^{1} f(x)\,dx = 2\sum_{i=0}^{(k-1)/2} \frac{f^{(2i)}(0)}{(2i+1)!} + \sum_{j=1}^{m} a_j\,[f^{(k)}(x_j) - f^{(k)}(-x_j)],\ k \text{ odd}$$

$$(2)\qquad \int_{-1}^{1} f(x)\,dx = 2\sum_{i=0}^{(k-2)/2} \frac{f^{(2i)}(0)}{(2i+1)!} + \sum_{j=1}^{m} a_j\,[f^{(k)}(x_j) + f^{(k)}(-x_j)],\ k \text{ even}$$

are given in table 2 for $k = 1, 2$, $m = 1(1)10$. Coefficients of related orthogonal polynomials are given in table 1 for $k = 1, 2$, $m = 0(1)11$. The remainder terms for formulas (1) and (2) are

$$(3)\qquad R_{k,m} = \begin{cases} \dfrac{f^{(4m+k+1)}(\eta)}{(4m+1)!}\, C_{k,m},\ k \text{ odd} \\[2ex] \dfrac{f^{(4m+k)}(\eta)}{(4m)!}\, C_{k,m},\ k \text{ even}. \end{cases}$$

The $C_{k,m}$ are listed in table 3, for the same k and m as in table 2.

2. Calculations. The polynomials $P_{m,k}(x)$ were generated by orthonormalization of the sequence $1, x, \cdots, x^m$ with weight functions

$$(4)\qquad W_k(x) = \begin{cases} \dfrac{(1-\sqrt{x})^k}{k!},\ k \text{ odd} \\[2ex] \dfrac{(1-\sqrt{x})^k}{k!\sqrt{x}},\ k \text{ even} \end{cases}$$

on the interval (0, 1). Their coefficients were obtained as solutions to systems of linear equations. The x_j are the square roots of the zeros r_j of $P_{m,k}(x)$. The numbers a_j are determined by

$$(5)\qquad a_j = \begin{cases} \dfrac{A_{m+1,k}}{2x_j\,P'_{m,k}(r_j)\,P_{m+1,k}(r_j)},\ k \text{ odd} \\[2ex] \dfrac{A_{m+1,k}}{2P'_{m,k}(r_j)\,P_{m+1,k}(r_j)},\ k \text{ even} \end{cases}$$

where $A_{m,k}$ is the quotient of leading coefficients of $P_{m,k}$ and $P_{m-1,k}$. The values of $C_{k,m}$ for use in the remainder terms were derived from

$$(6)\qquad C_{k,m} = \begin{cases} 2\left[\dfrac{(4m+1)!}{(4m+k+2)!} - \displaystyle\sum_{j=1}^{m} a_j\,x_j^{4m+1}\right],\ k \text{ odd} \\[2ex] 2\left[\dfrac{(4m)!}{(4m+k+1)!} - \displaystyle\sum_{j=1}^{m} a_j\,x_j^{4m}\right],\ k \text{ even}, \end{cases}$$

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TABLE 1

$k = 1$

$P_0 = 1.73205\ 08075\ 6888$

$P_1 = 7.53370\ 80350\ 0884x - 2.26011\ 24105\ 0265$

$P_2 = 30.89988\ 23741\ 862x^2 - 23.66207\ 20883\ 408x + 2.68435\ 27159\ 0420$

$P_3 = 125.09567\ 55614\ 90x^3 - 156.54342\ 49462\ 16x^2 + 49.95110\ 87256\ 310x - 3.04662\ 58269\ 2541$

$P_4 = 503.92224\ 31999\ 51x^4 - 878.56845\ 42019\ 08x^3 + 480.77283\ 44538\ 39x^2 - 87.74164\ 92632\ 052x + 3.36803\ 13248\ 0860$

$P_5 = 2025.03058\ 73957\ 9x^5 - 4532.89143\ 04158\ 0x^4 + 3554.73528\ 18164\ 0x^3 - 1152.71421\ 91499\ 2x^2 + 138.22772\ 15120\ 70x - 3.65996\ 50721\ 1686$

$P_6 = 8126.60217\ 35502\ x^6 - 22225.89230\ 7314x^5 + 22794.37521\ 9445x^4 - 10831.68147\ 2854x^3 + 2371.48444\ 08556\ x^2 - 202.49633\ 19667\ 4x + 3.92935\ 16425\ 271$

$P_7 = 32585.34917\ 364x^7 - 1\ 05329.15543\ 67x^6 + 1\ 33708.35590\ 97x^5 - 84369.53936\ 860x^4 + 27562.57790\ 493x^3 - 4390.47486\ 2558x^2 + 281.55199\ 51626x - 4.18076\ 36516\ 86$

$P_8 = 1\ 30585.72574\ x^8 - 4\ 87145.05832\ x^7 + 7\ 37945.40041\ x^6 - 5\ 82772.09740\ x^5 + 2\ 56072.42057\ x^4 - 61782.59435\ 9x^3 + 7521.30300\ 46x^2 - 376.33313\ 306x + 4.41740\ 68709$

$P_9 = 5\ 23121.399x^9 - 22\ 12241.35x^8 + 38\ 96351.95x^7 - 37\ 02822.37x^6 + 20\ 55853.62x^5 - 6\ 74493.559x^4 + 1\ 25947.128x^3 - 12137.5185x^2 + 487.72367\ 9x - 4.63163\ 193$

$P_{10} = 20\ 95022.5x^{10} - 99\ 04599.4x^9 + 198\ 92582.x^8 - 221\ 24981.x^7 + 148\ 91824.x^6 - 62\ 25087.3x^5 + 15\ 95661.1x^4 - 2\ 38415.82x^3 + 18678.058x^2 - 616.56109x + 4.85521\ 90$

$P_{11} = 83\ 88194.x^{11} - 438\ 42170.x^{10} + 989\ 11790.x^9 - 1261\ 15400.x^8 + 999\ 31000.x^7 - 509\ 73540.x^6 + 167\ 70010.x^5 - 34\ 68084.x^4 + 4\ 25177.7x^3 - 27649.29x^2 + 763.6075x - 5.05931\ 2$

$k = 2$

$P_0 = 1.73205\ 08075\ 6888$

$P_1 = 12.70977\ 81860\ 449x - 1.27097\ 78186\ 0449$

$P_2 = 59.88757\ 23920\ 599x^2 - 29.17599\ 68063\ 882x + 1.20652\ 61837\ 2282$

$P_3 = 259.32961\ 55268\ 10x^3 - 242.98324\ 64964\ 47x^2 + 50.37043\ 53148\ 982x - 1.18192\ 23907\ 2002$

$P_4 = 1087.36971\ 21542\ 1x^4 - 1531.67966\ 14027\ 7\ x^3 + 633.73798\ 31134\ 97x^2 - 76.31728\ 62592\ 196x + 1.16909\ 13241\ 5856$

$P_5 = 4487.70266\ 55197\ 8x^5 - 8483.52105\ 08986\ 2x^4 + 5405.81028\ 77031\ 0x^3 - 1335.91407\ 05265\ 8x^2 + 106.99341\ 52181\ 20x - 1.16124\ 14205\ 1600$

$P_6 = 18355.66707\ 8423x^6 - 43644.30820\ 7345x^5 + 37942.62659\ 3113x^4 - 14721.14915\ 1884x^3 + 2472.29781\ 31355\ x^2 - 142.37405\ 03369\ 3x + 1.15594\ 79227\ 687$

$P_7 = 74659.95872\ 219x^7 - 2\ 14151.18872\ 09x^6 + 2\ 36965.50353\ 31x^5 - 1\ 27161.63787\ 63x^4 + 34058.68565\ 087x^3 - 4184.54516\ 3429x^2 + 182.43804\ 37977x - 1.15213\ 67777\ 11$

$P_8 = 3\ 02544.85398\ 6x^8 - 10\ 16908.12494\ x^7 + 13\ 69647.20094\ x^6 - 9\ 45055.96574\ 0x^5 + 3\ 54167.19148\ 2x^4 - 70308.79999\ 50\ x^3 + 6633.07482\ 984x^2 - 227.16794\ 4900x + 1.14926\ 09079\ 5$

$P_9 = 12\ 22819.3856x^9 - 47\ 14584.9219x^8 + 74\ 930684.8783x^7 - 63\ 42588.4460x^6 + 30\ 83282.8184x^5 - 8\ 64946.91266x^4 + 1\ 33312.13054x^3 - 9996.98758\ 11x^2 + 276.54933\ 828x - 1.14701\ 28163$

$P_{10} = 49\ 33033.914x^{10} - 214\ 63128.26x^9 + 393\ 48240.15\ x^8 - 395\ 46800.17x^7 + 237\ 46979.27x^6 - 87\ 07972.887x^5 + 19\ 12893.189x^4 - 2\ 36576.7122x^3 + 14474.00552\ x^2 - 330.57026\ 87x + 1.14520\ 6765$

$P_{11} = 198\ 72572.1x^{11} - 963\ 24095.7x^{10} + 2001\ 94335.x^9 - 2332\ 57625.x^8 + 1672\ 30868.x^7 - 762\ 13570.1x^6 + 220\ 33307.3x^5 - 39\ 12962.35x^4 + 3\ 98072.797x^3 - 20280.6219\ x^2 + 389.22470\ 8x - 1.14373\ 626$

TABLE 2

m	j	k = 1	
		x_j	a_j
1	1	.5477225575 05166	.3042903097 25092
2	1	.3721456511 38755	.2998694151 77678
	2	.7920059217 60865	.0695342880 47154
3	1	.2820900214 17742	.2625168155 42158
	2	.6268601608 87658	.1158516504 33743
	3	.8825310979 63249	.0226513358 72470
4	1	.2273288824 80793	.2283023164 62706
	2	.5140806061 43694	.1313690234 71769
	3	.7563681074 02448	.0510204966 76312
	4	.9248839673 29570	.0093443207 77566
5	1	.1904841804 26525	.2005148719 02275
	2	.4344049427 27343	.1330163257 25257
	3	.6535558761 15115	.0693217404 15712
	4	.8292980447 85322	.0254519669 74067
	5	.9479286287 01912	.0045107921 65497
6	1	.1639811690 9936	.1782134815 8969
	2	.3756528865 1806	.1290409387 9439
	3	.5724366400 9800	.0790426562 2466
	4	.7417866536 8859	.0393058004 7950
	5	.8740336979 4142	.0139874045 8116
	6	.9618129567 5531	.0024324030 3689
7	1	.1439912886 45	.1601387035 18
	2	.3307098113 32	.1229802576 16
	3	.5079816905 42	.0833391819 77
	4	.6669327097 06	.0490821180 75
	5	.8006064071 09	.0237352491 28
	6	.9033361608 21	.0082842932 84
	7	.9708112198 58	.0014235185 93
8	1	.1283703842	.1452769503
	2	.2952852684	.1163542537
	3	.4559661731	.0844453524
	4	.6038699343	.0553533943
	5	.7338622714	.0318100298
	6	.8415994425	.0151045544
	7	.9235314840	.0052043396
	8	.9769705854	.0008871299
9	1	.115823631	.132878407
	2	.266673730	.109816541
	3	.413291816	.083725810
	4	.550684038	.059056710
	5	.674964515	.037887335
	6	.782771237	.021412447
	7	.871235919	.010039513
	8	.938022434	.003428033
	9	.981369607	.000581047
10	1	.10552258	.12239571
	2	.24309589	.10363706
	3	.37773918	.08198747
	4	.50552941	.06098113
	5	.62345737	.04220687
	6	.72888457	.02667176
	7	.81949694	.01489473
	8	.89332330	.00691990
	9	.94876470	.00234732
	10	.98461980	.00039623

TABLE 2—*Continued*

m	j	k = 2: x_j	k = 2: a_j
1	1	.3162277660 16838	.1666666666 66667
2	1	.2136036212 56443	.1437779500 85321
	2	.6644945298 23701	.0228887165 81346
3	1	.1638297723 39671	.1224797344 91539
	2	.5118494949 80572	.0395183540 10279
	3	.8050693913 12212	.0046685781 64849
4	1	.1336140770 13473	.1060360979 05865
	2	.4169305407 03968	.0469644870 94641
	3	.6739890075 18818	.0123633215 15102
	4	.8733068456 92833	.0013027601 51060
5	1	.1131072568 64736	.0933196598 68176
	2	.3520392516 58368	.0494739624 16079
	3	.5769763210 36054	.0188805340 81087
	4	.7683849647 09291	.0045407258 01483
	5	.9112358854 64930	.0004517844 99852
6	1	.0982014632 7176	.0832757144 1884
	2	.3048169927 4399	.0495578221 5891
	3	.5034255107 0724	.0234294328 9172
	4	.6810857911 4211	.0083180426 8343
	5	.8274681084 1897	.0019025149 7640
	6	.9344124389 0913	.0001831395 3766
7	1	.0868450485 199	.0751675980 885
	2	.2688827298 199	.0484760818 692
	3	.4461187708 020	.0263277958 602
	4	.6095094010 734	.0117357442 186
	5	.7517394338 839	.0039910960 716
	6	.8666985675 800	.0008849203 899
	7	.9495850305 493	.0000834301 748
8	1	.0778891768 89	.0684940996 00
	2	.2406041327 18	.0468585232 40
	3	.4003534653 41	.0280343978 67
	4	.5505429051 14	.0145005204 06
	5	.6858231067 44	.0062300015 19
	6	.8015939596 43	.0020600871 63
	7	.8940032842 24	.0004474372 29
	8	.9600499057 83	.0000415997 26
9	1	.0706369010 2	.0629090570 4
	2	.2177597386 8	.0450255142 4
	3	.3630238378 6	.0289225611 3
	4	.5014536828 7	.0166061935 8
	5	.6290237349 3	.0083212591 4
	6	.7422126043 9	.0034868683 1
	7	.8379675527 1	.0011308362 0
	8	.9137418873 3	.0002420894 9
	9	.9675684295 0	.0000222879 4
10	1	.0646394150	.0581677528
	2	.1989137370	.0431420181
	3	.3320234405	.0292595373
	4	.4601078372	.0181452843
	5	.5800614933	.0101353888
	6	.6891397684	.0049671598
	7	.7849102517	.0020445253
	8	.8652666620	.0006538257
	9	.9284600004	.0001385086
	10	.9731500562	.0000126607

TABLE 3*

$k = 1$		$k = 2$	
m	$C_{1,m}$	m	$C_{2,m}$
1	1.7619×10^{-2}	1	6.1905×10^{-3}
2	1.0473×10^{-3}	2	2.7882×10^{-4}
3	6.3902×10^{-5}	3	1.4869×10^{-5}
4	3.9380×10^{-6}	4	8.4576×10^{-7}
5	2.4386×10^{-7}	5	4.9654×10^{-8}
6	1.5142×10^{-8}	6	2.9680×10^{-9}
7	9.4185×10^{-10}	7	1.7940×10^{-10}
8	6.3112×10^{-11}	8	1.0922×10^{-11}
9	7.7×10^{-11}	9	6.8464×10^{-13}
10	-3.3×10^{-10}	10	-2.8×10^{-13}

* These figures include round-off errors.

and thus show effects of round-off errors in a_j and x_j as well as the theoretical remainder. Since the matrix of the linear system solved to find the coefficients of $P_{m,k}(x)$ is ill-conditioned, the accuracy of the figures decreases rapidly with increasing m. Figures are kept to the upper limit of accuracy. If results are rounded to one or two fewer significant figures than are carried in the table of x_j, there is no doubt of the accuracy of the digits kept.

The formulas were derived in [1]. The calculations were carried out in the Numerical Analysis Laboratory of the University of Wisconsin on the IBM 650. An 18-digit floating-decimal interpretive routine by Eugene Albright and a linear systems solver by Gerald Thorne were used. I am indebted to William Kammerer for several helpful suggestions.

University of Wisconsin
Madison, Wisconsin

1. P. C. HAMMER & H. H. WICKE, "Quadrature formulas involving derivatives of the integrand," *Math. Comp.* (*MTAC*), v. 14, 1960, p. 3–7.