Numerical Integration Constants

Tables of the b_j and x_j in the approximate quadrature formula

$$\int_0^1 x^n g(x)dx \doteq \sum_{j=1}^{m} b_j g(x_j) \tag{1}$$

are given for $n = 0(1)5$, $m = 1(1)8$ to 12D. The x_j are the zeros of certain orthonormal polynomials $q_m(x)$; the $q_m(x)$ are given explicitly for the same range of n, m. It is well known that there is equality in (1) for polynomials not exceeding degree $2m - 1$. These tables extend those given by Hammer, Marlowe, and Stroud [2].

P. C. Hammer points out that due to the relation,

$$\int_c^d \left\{ \left(\int_c^t \right)^n f(t)(dt)^n \right\} dt = \frac{(d-c)^{n+1}}{n!} \int_0^1 x^n f(d - [d-c]x)dx,$$

(see [4]), the tables given below can be applied to the evaluation of repeated integrals.

$n = 0$

m	
0	$q_0(x) = \sqrt{1}$
1	$q_1(x) = \sqrt{3}(1 - 2x)$
2	$q_2(x) = \sqrt{5}(1 - 6x + 6x^2)$
3	$q_3(x) = \sqrt{7}(1 - 12x + 30x^2 - 20x^3)$
4	$q_4(x) = \sqrt{9}(1 - 20x + 90x^2 - 140x^3 + 70x^4)$
5	$q_5(x) = \sqrt{11}(1 - 30x + 210x^2 - 560x^3 + 630x^4 - 252x^5)$
6	$q_6(x) = \sqrt{13}(1 - 42x + 420x^2 - 1680x^3 + 3150x^4 - 2772x^5 + 924x^6)$
7	$q_7(x) = \sqrt{15}(1 - 56x + 756x^2 - 4200x^3 + 11550x^4 - 16632x^5 + 12012x^6 - 3432x^7)$
8	$q_8(x) = \sqrt{17}(1 - 72x + 1260x^2 - 9240x^3 + 34650x^4 - 72072x^5 + 84084x^6 - 51480x^7 + 12870x^8)$.

$n = 1$

m	
0	$q_0(x) = \sqrt{2}$
1	$q_1(x) = \sqrt{4}(2 - 3x)$
2	$q_2(x) = \sqrt{6}(3 - 12x + 10x^2)$
3	$q_3(x) = \sqrt{8}(4 - 30x + 60x^2 - 35x^3)$
4	$q_4(x) = \sqrt{10}(5 - 60x + 210x^2 - 280x^3 + 126x^4)$
5	$q_5(x) = \sqrt{12}(6 - 105x + 560x^2 - 1260x^3 + 1260x^4 - 462x^5)$
6	$q_6(x) = \sqrt{14}(7 - 168x + 1260x^2 - 4200x^3 + 6930x^4 - 5544x^5 + 1716x^6)$
7	$q_7(x) = \sqrt{16}(8 - 252x + 2520x^2 - 11550x^3 + 27720x^4 - 36036x^5 + 24024x^6 - 6435x^7)$
8	$q_8(x) = \sqrt{18}(9 - 360x + 4620x^2 - 27720x^3 + 90090x^4 - 168168x^5 + 180180x^6 - 102960x^7 + 24310x^8)$

$n = 2$

0 $q_0(x) = \sqrt{3}$

1 $q_1(x) = \sqrt{5}(3 - 4x)$

2 $q_2(x) = \sqrt{7}(6 - 20x + 15x^2)$

3 $q_3(x) = \sqrt{9}(10 - 60x + 105x^2 - 56x^3)$

4 $q_4(x) = \sqrt{11}(15 - 140x + 420x^2 - 504x^3 + 210x^4)$

5 $q_5(x) = \sqrt{13}(21 - 280x + 1260x^2 - 2520x^3 + 2310x^4 - 792x^5)$

6 $q_6(x) = \sqrt{15}(28 - 504x + 3150x^2 - 9240x^3 + 13860x^4 - 10296x^5 + 3003x^6)$

7 $q_7(x) = \sqrt{17}(36 - 840x + 6930x^2 - 27720x^3 + 60060x^4 - 72072x^5 + 45045x^6 - 11440x^7)$

8 $q_8(x) = \sqrt{19}(45 - 1320x + 13860x^2 - 72072x^3 + 210210x^4 - 360360x^5 + 360360x^6 - 194480x^7 + 43758x^8)$

$n = 3$

0 $q_0(x) = \sqrt{4}$

1 $q_1(x) = \sqrt{6}(4 - 5x)$

2 $q_2(x) = \sqrt{8}(10 - 30x + 21x^2)$

3 $q_3(x) = \sqrt{10}(20 - 105x + 168x^2 - 84x^3)$

4 $q_4(x) = \sqrt{12}(35 - 280x + 756x^2 - 840x^3 + 330x^4)$

5 $q_5(x) = \sqrt{14}(56 - 630x + 2520x^2 - 4620x^3 + 3960x^4 - 1287x^5)$

6 $q_6(x) = \sqrt{16}(84 - 1260x + 6930x^2 - 18480x^3 + 25740x^4 - 18018x^5 + 5005x^6)$

7 $q_7(x) = \sqrt{18}(120 - 2310x + 16632x^2 - 60060x^3 + 120120x^4 - 135135x^5 + 80080x^6 - 19448x^7)$

8 $q_8(x) = \sqrt{20}(165 - 3960x + 36036x^2 - 168168x^3 + 450450x^4 - 720720x^5 + 680680x^6 - 350064x^7 + 75582x^8)$

$n = 4$

0 $q_0(x) = \sqrt{5}$

1 $q_1(x) = \sqrt{7}(5 - 6x)$

2 $q_2(x) = \sqrt{9}(15 - 42x + 28x^2)$

3 $q_3(x) = \sqrt{11}(35 - 168x + 252x^2 - 120x^3)$

4 $q_4(x) = \sqrt{13}(70 - 504x + 1260x^2 - 1320x^3 + 495x^4)$

5 $q_5(x) = \sqrt{15}(126 - 1260x + 4620x^2 - 7920x^3 + 6435x^4 - 2002x^5)$

6 $q_6(x) = \sqrt{17}(210 - 2772x + 13860x^2 - 34320x^3 + 45045x^4 - 30030x^5 + 8008x^6)$

7 $q_7(x) = \sqrt{19}(330 - 5544x + 36036x^2 - 120120x^3 + 225225x^4 - 240240x^5 + 136136x^6 - 31824x^7)$

8 $q_8(x) = \sqrt{21}(495 - 10296x + 84084x^2 - 360360x^3 + 900900x^4 - 1361360x^5 + 1225224x^6 - 604656x^7 + 125970x^8)$

$n = 5$

0 $q_0(x) = \sqrt{6}$

1 $q_1(x) = \sqrt{8}(6 - 7x)$

2 $q_2(x) = \sqrt{10}(21 - 56x + 36x^2)$

3 $q_3(x) = \sqrt{12}(56 - 252x + 360x^2 - 165x^3)$

4 $q_4(x) = \sqrt{14}(126 - 840x + 1980x^2 - 1980x^3 + 715x^4)$

5 $q_5(x) = \sqrt{16}(252 - 2310x + 7920x^2 - 12870x^3 + 10010x^4 - 3003x^5)$

6 $q_6(x) = \sqrt{18}(462 - 5544x + 25740x^2 - 60060x^3 + 75075x^4 - 48048x^5 + 12376x^6)$

7 $q_7(x) = \sqrt{20}(792 - 12012x + 72072x^2 - 225225x^3 + 400400x^4 - 408408x^5 + 222768x^6 - 50388x^7)$

8 $q_8(x) = \sqrt{22}(1287 - 24024x + 180180x^2 - 720720x^3 + 1701700x^4 - 2450448x^5 + 2116296x^6 - 1007760x^7 + 203490x^8)$

$n = 0$

m	j	x_j	b_j
1	1	.50000 00000 00	1.00000 00000 00
2	1	.21132 48654 05	.50000 00000 00
	2	.78867 51345 95	.50000 00000 00
3	1	.11270 16653 79	.27777 77777 78
	2	.50000 00000 00	.44444 44444 44
	3	.88729 83346 21	.27777 77777 78
4	1	.06943 18442 03	.17392 74225 69
	2	.33000 94782 08	.32607 25774 31
	3	.66999 05217 92	.32607 25774 31
	4	.93056 81557 97	.17392 74225 69
5	1	.04691 00770 31	.11846 34425 28
	2	.23076 53449 47	.23931 43352 50
	3	.50000 00000 00	.28444 44444 44
	4	.76923 46550 53	.23931 43352 50
	5	.95308 99229 69	.11846 34425 28
6	1	.03376 52428 98	.08566 22461 90
	2	.16939 53067 67	.18038 07865 24
	3	.38069 04069 58	.23395 69672 86
	4	.61930 95930 42	.23395 69672 86
	5	.83060 46932 33	.18038 07865 24
	6	.96623 47571 02	.08566 22461 90
7	1	.02544 60438 29	.06474 24830 84
	2	.12923 44072 00	.13985 26957 45
	3	.29707 74243 11	.19091 50252 53
	4	.50000 00000 00	.20897 95918 37
	5	.70292 25756 89	.19091 50252 53
	6	.87076 55928 00	.13985 26957 45
	7	.97455 39561 71	.06474 24830 84
8	1	.01985 50717 51	.05061 42681 45
	2	.10166 67612 93	.11119 05172 27
	3	.23723 37950 42	.15685 33229 39
	4	.40828 26787 52	.18134 18916 89
	5	.59171 73212 48	.18134 18916 89
	6	.76276 62049 58	.15685 33229 39
	7	.89833 32387 07	.11119 05172 27
	8	.98014 49282 49	.05061 42681 45

$n = 1$

m	j	x_j	b_j
1	1	.66666 66666 67	.50000 00000 00
2	1	.35505 10257 22	.18195 86182 56
	2	.84494 89742 78	.31804 13817 44
3	1	.21234 05382 39	.06982 69799 01
	2	.59053 31355 59	.22924 11063 60
	3	.91141 20404 87	.20093 19137 39
4	1	.13975 98643 44	.03118 09709 50
	2	.41640 95676 31	.12984 75476 08
	3	.72315 69863 62	.20346 45680 10
	4	.94289 58038 85	.13550 69134 31
5	1	.09853 50857 99	.01574 79145 22
	2	.30453 57266 46	.07390 88700 73
	3	.56202 51897 53	.14638 69870 85
	4	.80198 65821 26	.16717 46380 94
	5	.96019 01429 49	.09678 15902 27
6	1	.07305 43286 80	.00873 83018 14
	2	.23076 61379 70	.04395 51655 51
	3	.44132 84812 28	.09866 11508 91
	4	.66301 53097 19	.14079 25537 88
	5	.85192 14003 32	.13554 24972 32
	6	.97068 35728 40	.07231 03307 26
7	1	.05626 25605 37	.00521 43622 03
	2	.18024 06917 37	.02740 83567 22
	3	.35262 47171 13	.06638 46964 65
	4	.54715 36263 31	.10712 50656 96
	5	.73421 01772 15	.12739 08973 00
	6	.88532 09468 39	.11050 92581 91
	7	.97752 06135 61	.05596 73634 23
8	1	.04463 39552 90	.00329 51914 42
	2	.14436 62570 42	.01784 29026 56
	3	.28682 47571 44	.04543 93195 05
	4	.45481 33151 97	.07919 95994 92
	5	.62806 78354 17	.10604 73594 36
	6	.78569 15206 04	.11250 57994 71
	7	.90867 63921 00	.09111 90236 36
	8	.98222 00848 53	.04455 08043 62

$n = 2$

m	j	x_j	b_j
1	1	.75000 00000 00	.33333 33333 33
2	1	.45584 81559 89	.10078 58820 80
	2	.87748 51773 45	.23254 74512 54
3	1	.29499 77901 12	.02995 07030 09
	2	.65299 62339 62	.14624 62692 60
	3	.92700 59759 27	.15713 63610 65

m	j	x_j	b_j
4	1	.20414 85821 03	.01035 22407 50
	2	.48295 27048 96	.06863 38871 73
	3	.76139 92624 48	.14345 87897 99
	4	.95149 94505 53	.11088 84156 11
5	1	.14894 57870 53	.00411 38252 03
	2	.36566 65273 69	.03205 56007 23
	3	.61011 36129 34	.08920 01612 22
	4	.82651 96792 28	.12619 89619 00
	5	.96542 10600 82	.08176 47842 86
6	1	.11319 43838 22	.00183 10758 07
	2	.28431 88726 88	.01572 02971 85
	3	.49096 35868 35	.05128 95711 30
	4	.69756 30819 77	.09457 71867 49
	5	.86843 60583 42	.10737 64997 37
	6	.97409 54449 06	.06253 87027 27
7	1	.08881 68334 37	.00089 26880 34
	2	.22648 27534 09	.00816 29256 32
	3	.39997 84867 21	.02942 22112 90
	4	.58599 78554 03	.06314 63787 09
	5	.75944 58739 52	.09173 38032 80
	6	.89691 09708 52	.09069 88246 13
	7	.97986 72262 27	.04927 65017 76
8	1	.07149 10350 40	.00046 85177 84
	2	.18422 82964 17	.00447 45217 13
	3	.33044 77281 76	.01724 68637 80
	4	.49440 29218 16	.04081 44263 89
	5	.65834 80085 23	.06844 71834 22
	6	.80452 48315 11	.08528 47691 72
	7	.91709 93825 14	.07681 80932 67
	8	.98390 22404 48	.03977 89578 07

$n = 3$

m	j	x_j	b_j
1	1	.80000 00000 00	.25000 00000 00
2	1	.52985 79358 95	.06690 52498 07
	2	.89871 34926 77	.18309 47501 93
3	1	.36326 46302 17	.01647 90592 83
	2	.69881 12691 64	.10459 98975 57
	3	.93792 41006 20	.12892 10431 61
4	1	.26147 77888 31	.00465 83670 60
	2	.53584 64460 88	.04254 17241 43
	3	.79028 32299 69	.10900 43689 39
	4	.95784 70805 66	.09379 55398 59
5	1	.19621 20073 97	.00152 06893 71
	2	.41710 02118 22	.01695 73248 63
	3	.64857 00042 37	.06044 49532 04
	4	.84560 51499 74	.10031 65044 65
	5	.96943 57034 93	.07076 05280 97

m	j	x_j	b_j
6	1	.15227 31617 84	.00056 17108 74
	2	.33130 04570 38	.00708 53159 32
	3	.53241 15667 29	.03052 61922 26
	4	.72560 27783 30	.06844 32817 68
	5	.88161 66844 37	.08830 09912 41
	6	.97679 53516 82	.05508 25079 60
7	1	.12142 71288 32	.00022 99041 27
	2	.26836 34403 11	.00314 75964 07
	3	.44086 64606 23	.01531 21671 26
	4	.61860 40284 32	.04099 51686 04
	5	.78025 35519 66	.06975 00981 07
	6	.90636 25341 45	.07655 65613 63
	7	.98176 99145 14	.04400 85042 65
8	1	.09900 17577 10	.00010 24600 78
	2	.22124 35073 50	.00148 56840 83
	3	.36912 39000 12	.00785 50738 41
	4	.52854 54312 02	.02363 15806 68
	5	.68399 32484 32	.04745 43798 12
	6	.82028 39496 79	.06736 18393 93
	7	.92409 37128 99	.06618 20353 22
	8	.98529 34400 85	.03592 69468 03

$n = 4$

m	j	x_j	b_j
1	1	.83333 33333 33	.20000 00000 00
2	1	.58633 65823 23	.04908 24922 78
	2	.91366 34176 77	.15091 75077 22
3	1	.42011 30593 37	.01046 90421 83
	2	.73388 93552 08	.08027 66734 56
	3	.94599 75854 55	.10925 42843 61
4	1	.31213 54928 47	.00251 63516 47
	2	.57891 56595 62	.02916 93821 62
	3	.81289 15166 16	.08706 77120 64
	4	.96272 39976 41	.08124 65541 27
5	1	.23979 20448 02	.00069 69770 78
	2	.46093 36745 32	.01021 05417 25
	3	.68005 92327 41	.04402 44695 05
	4	.86088 63436 76	.08271 27131 02
	5	.97261 44185 34	.06235 52985 89
6	1	.18946 95839 22	.00021 94139 95
	2	.37275 11560 14	.00372 67844 39
	3	.56757 23728 55	.01995 62646 93
	4	.74883 64975 06	.05223 99542 93
	5	.89238 51584 47	.07464 91503 13
	6	.97898 52312 56	.04920 84322 67

m	j	x_j	b_j
7	1	.15324 14388 69	.00007 70737 07
	2	.30632 65225 42	.00144 70087 89
	3	.47654 00930 01	.00892 69676 13
	4	.64638 93025 20	.02854 78427 53
	5	.79771 66898 15	.05522 48741 64
	6	.91421 99005 65	.06602 18459 35
	7	.98334 38304 67	.03975 43870 40
8	1	.12637 29743 78	.00002 97092 30
	2	.25552 90520 78	.00059 89500 38
	3	.40364 12988 94	.00407 79241 35
	4	.55831 66757 90	.01490 99334 50
	5	.70600 95428 83	.03471 99506 61
	6	.83367 15420 39	.05491 00972 91
	7	.92999 57160 53	.05800 05652 68
	8	.98646 31978 85	.03275 28699 27

$n = 5$

m	j	x_j	b_j
1	1	.85714 28571 43	.16666 66666 67
2	1	.63079 15938 30	.03833 75627 37
	2	.92476 39617 26	.12832 91039 30
3	1	.46798 32354 55	.00729 70036 38
	2	.76162 39696 99	.06459 66122 96
	3	.95221 09766 64	.09477 30507 33
4	1	.35689 37290 50	.00153 44797 48
	2	.61466 93898 55	.02142 84046 31
	3	.83107 90038 60	.07205 63641 65
	4	.96658 86464 65	.07164 74181 22
5	1	.27969 31248 12	.00036 97154 99
	2	.49870 98270 30	.00672 96904 30
	3	.70633 38189 21	.03376 77449 58
	4	.87340 27278 72	.07007 13397 05
	5	.97519 38346 98	.05572 81760 75
6	1	.22446 89954 04	.00010 13258 20
	2	.40953 33504 56	.00218 79256 55
	3	.59778 90484 17	.01396 96530 85
	4	.76841 36046 08	.04148 63469 81
	5	.90135 07338 49	.06445 88591 64
	6	.98079 72084 41	.04446 25559 61
7	1	.18382 87683 01	.00003 11046 06
	2	.34080 75951 06	.00075 53838 32
	3	.50794 05240 29	.00566 04137 04
	4	.67036 34101 11	.02095 92981 75
	5	.81258 84659 90	.04510 49815 82
	6	.92085 64172 55	.05790 76135 39
	7	.98466 74507 86	.03624 78712 29

m	j	x_j	b_j
8	1	.15315 06616 10	.00001 05316 45
	2	.28726 44038 84	.00027 83586 15
	3	.43462 74066 99	.00233 53415 00
	4	.58451 85665 63	.01004 46143 88
	5	.72512 64097 13	.02648 53011 18
	6	.84518 94879 31	.04588 56532 01
	7	.93504 35074 56	.05153 42238 32
	8	.98746 05085 24	.03009 26423 68

The polynomials $q_i(x)$ are obtained by orthonormalization of the sequence $1, x, x^2, \cdots$ with weight function x^n in the interval (0, 1). The Jacobi polynomials are defined by Courant and Hilbert [1] as follows:

$$J_{m,n} = \frac{n!}{(m+n)!} x^{-n} \frac{d^m}{dx^m} x^{m+n}(1-x)^m.$$

(Editor's note. The author's $J_{m,n}(x)$ is Courant's $G_m(n+1, n+1, x)$, and this, except for a normalizing factor, is $P_m^{(n,0)}(2x-1)$ of the Bateman Project [3].) Since [1] we have

$$\int_0^1 x^n J_{k,n} J_{m,n} dx = \frac{1}{(n+2m+1)\binom{m+n}{n}^2} \delta_{k,m},$$

the corresponding orthonormal sequence is

$$q_m(x) = \sqrt{n+2m+1}\binom{m+n}{n} J_{m,n}(x)$$

$$= \sqrt{n+2m+1} \sum_{k=0}^{m} (-1)^k \binom{m+n+k}{m}\binom{m}{k} x^k.$$

The explicit formula for b_j is

$$b_j = \{\sum_{i=0}^{m-1} [q_i(x_j)]^2\}^{-1}.$$

Within the range of values given in tables I, II, III of the Hammer, Marlowe, Stroud paper, it is seen that these polynomials are identical to those given therein except for a factor of -1 in the ones of odd degree associated with weight function x^2. Obviously, this has no effect on the values in the table.

The Newton-Raphson method with synthetic division was used to find the zeros. With the polynomials of higher degree (*i.e.*, for $m = 6$, 7, and 8) and especially for the higher values of n where the coefficients are large, the round-off errors in the zeros for 18 decimal places were seen to be considerable. As a check these preliminary values were substituted back into the original equation and the process was carried out again with the zeros recorded after each iteration.

Synthetic division was not used this time because it was felt that the round-off error would be carried into the reduced polynomial. Observing the erratic property of the last digits it was concluded that the limit of accuracy in the worst case is about 12 decimal places. There seems to be no question for values of m from 1 to 5 where $n = 0$, 1, and 2.

A check of the b_j was made through the fact that

$$\sum_{j=1}^{m} b_j = \int_0^1 x^n dx = \frac{1}{n+1}$$

for each polynomial of degree m associated with x^n. Here again the limit of accuracy is put at about the twelfth decimal place for the worst possible cases (*i.e.*, with m and n both large). If one wishes to round off values to ten or eleven decimal places there should be no doubt of the accuracy.

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HERBERT FISHMAN

University of Wisconsin
Madison, Wisconsin

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Tables of the Exponential Integral Ei(x)

In some molecular structure calculations it is desirable to have values of the integral Ei(x) to higher accuracy than is provided by the standard tables [1]. Direct computation of the values needed is extremely tedious over a wide range of the argument intermediate between the regions where expansions about zero and infinity are useful. However, if a net of sufficiently accurate values of Ei(x) has already been computed, then the generation of additional values intermediate between these becomes a problem of a considerably lesser magnitude. A few such values have been published [2, 3]. Kotani [4] has given a considerable number of values in his most valuable compilation, but unfortunately they are of somewhat fewer significant figures than under discussion here. A prohibitive amount of labor would be required to make such an extensive accurate table that only simple interpolation formulas need be used. However, a most useful intermediate objective could be achieved if a table were prepared with entries sufficiently closely