Numerical Integration Over a Sphere*

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1. Introduction. Peirce [5] has developed a method of determining numerical integration formulas of arbitrarily high polynomial accuracy for the integration of functions over a spherical shell of outer radius unity and inner radius R, $0 \leqq R < 1$. The purpose of this paper is to provide, for the special case $R = 0$, the zeros and weight coefficients of the Jacobi polynomials $G_{m+1}(3/2, 3/2, x)$ necessary to perform integrations of accuracy $4m + 3$, $m = 0(1)25$ (see microfiche card for this issue). For this case these formulas are of general interest, for they may be extended to apply to arbitrary ellipsoids by application of a theorem given by Hammer and Wymore [3]. A brief summary of the pertinent results of these authors is given with a discussion of the determination of the numerical data. Table I contains the zeros and weight coefficients of $G_{m+1}(3/2, 3/2, x)$ to 20D.

TABLE I
The roots r_k and weights C_k of $G_{m+1}(3/2, 3/2, r^2)$, $m = 0(1)14$

$m = 0$		
	0.33333333333333333333	0.77459666924148337704
$m = 1$		
	0.13877799911553081507	0.53846931010568309104
	0.19455533421780251827	0.90617984593866399280
$m = 2$		
	0.06289133716441942398	0.40584515137739716691
	0.15380118384095636775	0.74153118559939443986
	0.11664081232795754160	0.94910791234275852453
$m = 3$		
	0.03284025994586209607	0.32425342340380892904
	0.09804813271549816746	0.61337143270059039731
	0.12626367286460207059	0.83603110732663579430
	0.07618126780737099922	0.96816023950762608984
$m = 4$		
	0.01909367337020706716	0.26954315595234497233
	0.06283657634659116753	0.51909612920681181593
	0.09931540074741397873	0.73015200557404932409
	0.09881668814540756267	0.88706259975809529908
	0.05327099472371355724	0.97822865814605699280
$m = 5$		
	0.01201813399575544179	0.23045831595513479407
	0.04180131427256623277	0.44849275103644685288
	0.07350528946306196213	0.64234933944034022064
	0.08923004038646593360	0.80157809073330991279
	0.07756508890987825666	0.91759839922297796521
	0.03921346630560550638	0.98418305471858814947

Received July 31, 1967.

* Research sponsored by Office of Research Analyses, Office of Aerospace Research, United States Air Force.

TABLE I—*Continued*

$m = 6$		
	0.00803232068690877698	0.20119409399743452230
	0.02892109510217531901	0.39415134707756336990
	0.05420529441321764964	0.57097217260853884754
	0.07324404684277204383	0.72441773136017004742
	0.07709617353803761699	0.84820658341042721620
	0.06181526476141266936	0.93727339240070590431
	0.03001913798880925752	0.98799251802048542849
$m = 7$		
	0.00562468801729387511	0.17848418149584785585
	0.02072561633610808330	0.35123176345387631530
	0.04049117274162919867	0.51269053708647696789
	0.05845071638312108904	0.65767115921669076585
	0.06833464151929247110	0.78151400389680140693
	0.06588779073318947860	0.88023915372698590212
	0.05012343239466934894	0.95067552176876776122
	0.02369527520802978857	0.99057547531441733568
$m = 8$		
	0.00408786715295897713	0.16035864564022537587
	0.01530911730948734674	0.31656409996362983199
	0.03077823035884102378	0.46457074137596094572
	0.04643571696325461523	0.60054530466168102347
	0.05799147535563555918	0.72096617733522937862
	0.06192588169771199736	0.82271465653714282498
	0.05631898354194563146	0.90315590361481790164
	0.04131870342873501443	0.96020815213483003085
	0.01916735752476316801	0.99240684384358440319
$m = 9$		
	0.00306221969230961993	0.14556185416089509094
	0.01160453774144147563	0.28802131680240109660
	0.02381716978478938446	0.42434212020743878357
	0.03707127020662006787	0.55161883588721980706
	0.04842286915539797962	0.66713880419741231931
	0.05517892994515819127	0.76843996347567790862
	0.05541831208367090112	0.85336336458331728365
	0.04836902098033242550	0.92009933415040082879
	0.03457129606595389660	0.96722683856630629432
	0.01581770767765939134	0.99375217062038950026
$m = 10$		
	0.00235217893116765504	0.13325682429846611093
	0.00899345033491989197	0.26413568097034493053
	0.01874466998833659637	0.39030103803029083142
	0.02985217976107179918	0.50950147784600754969
	0.04026979394884106878	0.61960987576364615639
	0.04798859174890280536	0.71866136313195019446
	0.05136209309368605918	0.80488840161883989215
	0.04937512175927138489	0.87675235827044166738
	0.04181367314004632102	0.93297108682601610235
	0.02930966008147306769	0.97254247121811523196
	0.01327192054561668385	0.99476933499755212352

$m = 11$		
	0.00184533924279393446	0.12286469261071039639
	0.00710416051932268695	0.24386688372098843205
	0.01498273551830031569	0.36117230580938783774
	0.02427926747384041894	0.47300273144571496052
	0.03354828933252705568	0.57766293024122296772
	0.04129876262496723697	0.67356636847346836449
	0.04619908045399318128	0.75925926303735763058
	0.04726123753596655201	0.83344262876083400142
	0.04397924765379093931	0.89499199787827536885
	0.03640314079676698899	0.94297457122897433941
	0.02513929474244176331	0.97666392145951751150
	0.01129277743862225975	0.99555696979049809791
$m = 12$		
	0.00147402939756673698	0.11397258560952996693
	0.00570545527922939536	0.22645936543953685886
	0.01214471743450865018	0.33599390363850889973
	0.01994802619089263388	0.44114825175002688059
	0.02807674120313044230	0.54055156457945689490
	0.03541988576007397334	0.63290797194649514093
	0.04092552495593675894	0.71701347373942369929
	0.04372570002475941748	0.79177163907050822714
	0.04324035792738032477	0.85620790801829449030
	0.03924816550927529180	0.90948232067749110430
	0.03191601501357128716	0.95090055781470500685
	0.02178445431538310569	0.97992347596150122286
	0.00972426032162531546	0.99617926288898856694
$m = 13$		
	0.00119587775733535152	0.10627823013267923017
	0.00464893278792393988	0.21135228616600107451
	0.00996920386896910514	0.31403163786763993495
	0.01655127162320249233	0.41315288817400866389
	0.02363628891190294954	0.50759295512422764210
	0.03038983047823062825	0.59628179713822782038
	0.03598767131772407669	0.67821453760268651516
	0.03970079787631620966	0.75246285173447713391
	0.04097103149004312028	0.81818548761525244499
	0.03946959317891516767	0.87463780492010279042
	0.03513267329126566488	0.92118023295305878509
	0.02817045523520854148	0.95728559577808772580
	0.01904926947146495301	0.98254550526141317487
	0.00846043604483113302	0.99667944226059658616
$m = 14$		
	0.00098344490240772972	0.09955531215234152033
	0.00383662234147764057	0.19812119933557062877
	0.00827679050738779697	0.29471806998170161662
	0.01386103637144506918	0.38838590160823294306
	0.02002611137451000435	0.47819378204490248044
	0.02613914514789316859	0.56324916140714926272
	0.03155472455505853202	0.64270672292426034618
	0.03567325804468674171	0.71577678458685328391
	0.03799542959186337271	0.78173314841662494041
	0.03816789294734916700	0.83992032014626734009
	0.03601613586539902103	0.88976002994827104337
	0.03156159181196682479	0.93075699789664816496
	0.02502152825460420497	0.96250392509294966179
	0.01679224453034429409	0.98468590966515248400
	0.00742737708693976563	0.99708748181947707406

2. Peirce's Results. Peirce has shown that if the integral on the spherical shell of outer radius unity and inner radius R of the function $f(x, y, z)$, defined and continuous on the shell, is transformed by

$$x = r \sin \phi \cos \theta ,$$
$$y = r \sin \phi \sin \theta ,$$
$$z = r \cos \phi ,$$

to spherical coordinates, the resulting integral

$$I = \int_R^1 \int_0^\pi \int_0^{2\pi} r^2 \sin \phi F(\theta, \varphi, r) d\theta d\varphi dr$$

may be approximated by a formula of the form

$$\sum_i \sum_j \sum_k A_i B_j C_k F(\theta_i, \phi_j, r_k)$$

where $F(\theta, \phi, r) = f(r \sin \phi \cos \theta, r \sin \phi \sin \theta, r \cos \phi)$ and the A_i, B_j, C_k are constants.

In particular, he showed that a formula of accuracy $s = 4m + 3$ in $r \sin \phi \cos \theta$, $r \sin \phi \sin \theta$, $r \cos \phi$, $m = 0, 1, \cdots$ results if

(a) $\theta_i = 2\pi i/(s + 1)$, $i = 1, 2, \cdots, s + 1$;

(b) the $\cos \phi_j$ are the $2m + 2$ zeros of the Legendre polynomial of degree $2m + 2$, P_{2m+2}, orthogonalized on $[-1, 1]$;

(c) the r_k^2 are the zeros of the polynomial in r^2 of degree $m + 1$, $Q_{m+1}(r^2)$, where

$$\int_R^1 r^2 Q_{m+1}(r^2) T_m(r^2) dr = 0 , \tag{2.1}$$

$T_m(r^2)$ being an arbitrary polynomial in r^2 of degree less than or equal to m, and

$$A_i = 2\pi/(s + 1) , \qquad i = 1, 2, \cdots, s + 1 ,$$
$$B_j = \frac{1}{P'_{2m+2}(x_j)} \int_{-1}^1 \frac{P_{2m+2}(x)}{x - x_j} dx , \qquad j = 1, 2, \cdots, 2m + 2 ,$$
$$C_k = \frac{1}{Q'_{m+1}(r_k^2)} \int_R^1 \frac{r^2 Q_{m+1}(r^2)}{r^2 - r_k^2} dr , \qquad k = 1, 2, \cdots, m + 1 ,$$

where $x_j = \cos \phi_j$, and $Q_{m+1}(r^2)$ indicates a derivative with respect to r^2.

3. Calculation of the Numerical Data. The extensive tables of the zeros and weight coefficients of the Legendre polynomials compiled by Davis and Rabinowitz [1] and Gawlik [2] are sufficient to cover the range of m under discussion. We are concerned, therefore, only with the zeros and weight coefficients of the $Q_{m+1}(r^2)$, $m = 0(1)25$. In general it has been shown by Mustard [4] that the polynomials determined from the conditions

$$\int_0^1 r^{n-1} Q_{m+1}(r^2) T_m(r^2) dr = 0 ,$$

where $T_m(r^2)$ is an arbitrary polynomial of degree m or less in r^2, are the Jacobi polynomials $G_{m+1}(n/2, n/2, r^2)$. By a straightforward manipulation of the hypergeometric series

$$F(\alpha, \beta, \gamma, x) = 1 + \frac{\alpha\beta}{1\cdot\gamma} x + \frac{\alpha(\alpha+1)\beta(\beta+1)}{1\cdot 2\gamma(\gamma+1)} x^2 + \cdots$$

where $\alpha = n/2 + m + 1$, $\beta = -(m+1)$, and $\gamma = n/2$, these polynomials may be written in a form convenient for computation, viz.,

$$Q_{m+1}(r^2) = (r^2)^{m+1} + \sum_{k=0}^{m} \left[(-1)^{m-k+1} \binom{m+1}{k} \prod_{j=k+1}^{m+1} \frac{2j + (n-2)}{2(m+j) + n} \right] (r^2)^k .$$

For the case of interest, $n = 3$, these are the $Q_{m+1}(r^2)$ of (2.1) with $R = 0$. The zeros were determined by synthetic division. The C_k were determined with the aid of the expansion

$$\int_0^1 \frac{r^2 Q_{m+1}(r^2)}{r^2 - r_k^2}\, dr = \sum_{i=0}^{m} \left[\sum_{k=0}^{i} b_{m+1-k} (r^2)^{i-k} \right] \frac{1}{2(m-i)+3}$$

where b_j is the coefficient of $(r^2)^j$ in $Q_{m+1}(r^2)$. Table I contains the r_k and C_k to 20D for $m = 0(1)14$ in the text, and for $m = 0(1)25$, on the microfiche card in this issue. Both quantities have been rounded. The accuracy of the results was checked by means of the relations

$$\sum r_k^2 = b_m , \qquad \sum b_k = 1/3 .$$

The checks indicate that the quantities are in error by at most ± 0.5 in the final digit. The computations were done in triple precision on a CDC 3600 using an arithmetic package prepared at Argonne National Laboratory. The θ_i and A_i are not given because they are easily calculated.

4. Extension of Peirce's Formula to an Arbitrary Ellipsoid. Using the results of Hammer and Wymore, a formula of accuracy $s = 4m + 3$ for the integration of a function over an arbitrary ellipsoid may be derived from Peirce's formula of corresponding accuracy. If we consider an ellipsoid with semiaxes, a, b, c, then the formula for the integration of a function f defined and continuous on the ellipsoid has the form

$$\sum_i \sum_j \sum_k abcA_i B_j C_k f(ar_k \sin\phi_j \cos\theta_i, br_k \sin\phi_j \sin\theta_i, cr_k \cos\phi_j) ,$$

where all quantities are as previously defined.

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1. P. Davis & P. Rabinowitz, "Abscissas and weights for Gaussian quadratures of high order," *J. Res. Nat. Bur. Standards*, v. 56, 1956, pp. 35–37. (See *MTAC*, v. 11, 1957, p. 209, RMT **84**.) MR **17**, 902.

2. H. J. Gawlik, *Zeros of Legendre Polynomials of Orders 2–64 and Weight Coefficients of Gauss Quadrature Formulae*, Armament Research and Development Establishment Memorandum (B) 77/58, Fort Halstead, Kent, December, 1958. (See *Math. Comp.*, v. 14, 1960, p. 77, RMT **4**.)

3. P. C. Hammer & A. W. Wymore, "Numerical evaluation of multiple integrals. I," *MTAC*, v. 11, 1957, pp. 59–67. MR **19**, 323.

4. D. Mustard, "Numerical integration over the n-dimensional spherical shell," *Math. Comp.*, v. 18, 1964, pp. 578–589. MR **30** #712.

5. W. H. Peirce, "Numerical integration over the spherical shell," *MTAC*, v. 11, 1957, pp. 244–249. MR **20** #430.