

Numerical Integration Over a Sphere*

By Christopher A. Feuchter

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 , $0 \leq R < 1$. 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 $G_{m+1}(3/2, 3/2, r^2)$, $m = 0(1)14$

$m = 0$	0.33333333333333333333333333333333	0.77459666924148337704
$m = 1$	0.13877799911553081507 0.19455533421780251827	0.53846931010568309104 0.90617984593866399280
$m = 2$	0.06289133716441942398 0.15380118384095636775 0.11664081232795754160	0.40584515137739716691 0.74153118559939443986 0.94910791234275852453
$m = 3$	0.03284025994586209607 0.09804813271549816746 0.12626367286460207059 0.07618126780737099922	0.32425342340380892904 0.61337143270059039731 0.83603110732663579430 0.96816023950762608984
$m = 4$	0.01909367337020706716 0.06283657634659116753 0.09931540074741397873 0.09881668814540756267 0.05327099472371355724	0.26954315595234497233 0.51909612920681181593 0.73015200557404932409 0.88706259975809529908 0.97822865814605699280
$m = 5$	0.01201813399575544179 0.04180131427256623277 0.07330528946306196213 0.08923004038646593360 0.07756508890987825666 0.03921346630560550638	0.23045831595513479407 0.44849275103644685288 0.64234933944034022064 0.80157809073330991279 0.9175983992297796521 0.98418305471858814947

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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	0.21135228616600170451
0.00996920386896910514	0.314031637867630993495
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

$$\begin{aligned}x &= r \sin \phi \cos \theta, \\y &= r \sin \phi \sin \theta, \\z &= r \cos \phi,\end{aligned}$$

to spherical coordinates, the resulting integral

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

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 $r \sin \phi \cos \theta, r \sin \phi \sin \theta, r \cos \phi, m = 0, 1, \dots$ results if

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

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

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

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

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

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

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

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

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

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

where all quantities are as previously defined.

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0.04180131427256623277
0.07350528946306196213
0.08923004038646593360
0.07756508890987825666
0.03921346630560550638

0.44849275103
0.64234933944
0.80157809073
0.91759839922
0.98418305471

m = 6

0.00803232068690877698
0.02892109510217531901
0.05420529441321764964
0.07324404684277204383
0.07709617353803761699
0.06181526476141266936
0.03001913798880925752

0.20119409399
0.39415134707
0.57097217260
0.72441773136
0.84820658341
0.93727339240
0.98799251802

m = 7

0.00562468801729387511
0.02072561633610808330
0.04049117274162919867
0.05845071638312108904
0.06833464151929247110
0.06588779073318947860
0.05012343239466934894
0.02369527520802978857

0.178484181495
0.351231763453
0.512690537086
0.657671159216
0.781514003896
0.880239153726
0.950675521768
0.990575475314

m = 8

0.00408786715295897713
0.01530911730948734674
0.03077823035884102378
0.04643571696325461523
0.05799147535563555918
0.06192588169771199736
0.05631898354194563146
0.04131870342873501443
0.01916735752476316801

0.160358645640
0.316564099963
0.464570741375
0.600545304661
0.720966177335
0.822714656537
0.903155983614
0.960208152134
0.992406843843

m = 9

0.00306221969230961993

0.145561854160

0.01160453774144147563
0.02381716978478938446
0.03707127020662006787
0.04842286915539797962
0.05517892994515819127
0.05541831208367090112
0.04836902098033242550
0.03457129606595389660
0.01581770767765939134

0.288021316802
0.424342120207
0.551618835887
0.667138804197
0.768439963475
0.853363364583
0.920099334150
0.967226838566
0.993752170620

m = 10

0.00235217893116765504
0.00899349033491989197
0.01874466998833659637
0.02985217976107179918
0.04026979394884106878
0.04798859174890280536
0.05136209309368605918
0.04937512175927138489
0.04181367314004632102
0.02930966008147306769
0.01327192054561668385

0.133256824298
0.264135680970
0.390301038030
0.509501477846
0.619609875763
0.718661363131
0.804888401618
0.876752358270
0.932971086826
0.972542471218
0.994769334997

m = 11

0.00184533924279393446
0.00710416051932268695
0.01498273551830031569
0.02427926747384041894
0.03354828933252705568
0.04129876262496723697
0.04619908045399318128
0.04726123753596655201
0.04397924765379093931
0.03640314079676698899
0.02513929474244176331
0.01129277743862225975

0.122864692610
0.243866883720
0.361172305809
0.473002731445
0.577662930241
0.673566368473
0.759259263037
0.833442628760
0.894991997878
0.942974571228
0.976663921459
0.995556969790

m = 12

0.00147402939756673698
0.00570545527922939536
0.01214471743450865018

0.113972585609
0.226459365439
0.335993903638

0.01994802619089263388
0.02807674120313044230
0.03541988576007397334
0.04092552495593675894
0.04372570002475941748
0.04324035792738032477
0.03924816550927529180
0.03191601501357128716
0.02178445431538310569
0.00972426032162531546

0.44114825175
0.54055156457
0.63290797194
0.71701347373
0.79177163907
0.85620790801
0.90948232067
0.95090055781
0.97992347596
0.99617926288

m = 13

0.00119587775733535152
0.00464893278792393988
0.00996920386896910514
0.01655127162320249233
0.02363628891190294954
0.03038983047823062825
0.03598767131772407669
0.03970079787631620966
0.04097103149004312028
0.03946959317891516767
0.03513267329126566488
0.02817045523520854148
0.01904926947146495301
0.00846043604483113302

0.10627823013
0.21135228616
0.31403163786
0.41315288817
0.50759295512
0.59628179713
0.67821453760
0.75246285173
0.81818548761
0.87463780492
0.92118023295
0.95728559577
0.98254550526
0.99667944226

m = 14

0.00098344490240772972
0.00383662234147764057
0.00827679050738779697
0.01386103637144506918
0.02002611137451000435
0.02613914514789316859
0.0315547245505853202
0.03567325804468674171
0.03799542959186337271
0.03816789294734916700
0.03601613586539902103
0.03156159181196682479
0.02502152825460420497
0.01679224453034429409
0.00742737708693976563

0.09955531215
0.19812119933
0.29471806998
0.38838590160
0.47819378204
0.56324916140
0.64270672292
0.71577678458
0.78173314841
0.83992032014
0.88976002994
0.93075699789
0.96250392509
0.98468590966
0.99708748181

m = 15

$m = 15$

0.00081843492151108188
0.00320219404520068952
0.00694232926655885143
0.01170910860753225009
0.01707825620775202990
0.02256474773224870113
0.02766150007453185172
0.03187990838727951884
0.03478903728649081023
0.03605037812104866705
0.03544543246774948655
0.03289394710833750328
0.02846136815089721228
0.02235497580925773585
0.01490946959869729557
0.00657224554823964802

0.0936310658
0.1864392988
0.2776090971
0.3663392577
0.4518500172
0.5333899047
0.6102423458
0.6817319599
0.7472304964
0.8061623562
0.8580096526
0.9023167677
0.9386943726
0.9668229096
0.9864557262
0.9974246942

$m = 16$

0.00068833297108225542
0.00269971315171573492
0.00587708358145087957
0.00997108024152360997
0.01465771420806416185
0.01956136416451396245
0.02428146591834513975
0.02842102590737289127
0.03161495729804755496
0.03355624919227016344
0.03401813090108303135
0.03287067381909629868
0.03009066435798048446
0.02576405963759537966
0.02008089856157790149
0.01332344155135265034
0.00585647787026123376

0.0883713432
0.1760510611
0.2623529412
0.3466015544
0.4281375415
0.5063227732
0.5805453447
0.6502243646
0.7148145015
0.7738102522
0.8267498990
0.8732191250
0.9128542613
0.9453451482
0.9704376160
0.9879357644
0.9977065690

$m = 17$

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Chebyshev Approximations for the Fresnel Integrals . . .	W. J. CODY	450
Approximations for the $x \exp x^2 \operatorname{erfc} x$ Function . . .	K. B. OLDHAM	454
REVIEWS AND DESCRIPTIONS OF TABLES AND BOOKS		455
BAILEY 35, RALSTON & WILF 36, BECKETT & HURT 37, ZUKHOVITSKIY & AVDEYEVA 38, WALSH 39, BERGER & DANSON 40, TOMPA 41, DORN & GREENBERG 42, DAVIS & RABINOWITZ 43, DEKANOSIDZE 44, CONCUS 45, MITRINOVIĆ 46, YUDIN & GOL'SHTEIN 47, SIMONNARD 48, HALE & LASALLE 49, MICHAUD 50, RICHTMYER & MORTON 51, NBS COMPUTATION LABORATORY 52, WYNDRUM & MITCHELL 53, ZHURINA & KARMAZINA 54, KERR 55, WALL 56, FOSTER 57, GOLDEN & LEICHUS 58, EDIE, HERMAN & ROTHERY 59, CHRETIEN & DESER 60		
TABLE ERRATA		472
ABRAMOWITZ & STEGUN 421, ERDÉLYI, MAGNUS, OBERHETTINGER & TRICOMI 422		
CORRIGENDA		474
JONES, LAL & BLUNDON, BARRODALE		
NOTE		475
Index of Government-Sponsored Computer Projects		

The editorial committee would welcome readers' comments about this microfiche feature. Please send comments to Professor Eugene Isaacson, MATHEMATICS OF COMPUTATION, Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, New York 10012.

Mathematics of Computation

TABLE OF CONTENTS

APRIL 1968

Construction of Gauss-Christoffel Quadrature Formulas	WALTER GAUTSCHI	251
Extensions of Symmetric Integration Formulas	A. H. STROUD	271
A Fast Fourier Transform Algorithm Using Base 8 Iterations	G. D. BERGLAND	275
Evaluation of Orthogonal Polynomials and Relationship to Evaluating Multiple Integrals	P. M. HIRSCH	280
An Error Analysis for Numerical Multiple Integration. II.	ROBERT E. BARNHILL	286
Numerical Integration Over a Sphere	CHRISTOPHER A. FEUCHTER	293
An Improved Method for the Numerical Solution of the Suspension Bridge Deflection Equations	R. W. DICKEY	298
Computation of Eigenvalues of Singular Sturm-Liouville Systems	D. O. BANKS & G. J. KUROWSKI	304
Convergence Rates of ADI Methods with Smooth Initial Error	ROBERT E. LYNCH & JOHN R. RICE	311
The Stability of Difference Approximations to a Self-Adjoint Parabolic Equation, Under Derivative Boundary Conditions	C. M. CAMPBELL & P. KEAST	336
Consistency Conditions for Difference Schemes with Singular Coefficients	DENNIS EISEN	347
Differentiation Formulas for Analytic Functions.	J. N. LYNNESS	352
Recursion Formulae for Hypergeometric Functions	JET WIMP	363
On Solving Systems of Equations Using Interval Arithmetic	ELDON R. HANSEN	374
Natural Sorting Over Permutation Spaces	R. M. BAER & P. BROCK	385
An Evaluation of Golomb's Constant	W. C. MITCHELL	411
TECHNICAL NOTES AND SHORT PAPERS		
Explicit Gap Series at Cusps of $\Gamma(p)$	A. O. L. ATKIN	416
A Report on Prime Numbers of the Forms $M = (6a + 1)2^{2m-1} - 1$ and $M' = (6a - 1)2^{2m} - 1$	H. C. WILLIAMS & C. R. ZARKE	420
Distribution of the Figures 0 and 1 in the Various Orders of Binary Repre- sentations of k th Powers of Integers	W. GROSS & R. VACCA	423
Explicit Inverses and Condition Numbers of Certain Circulants	S. CHARONMAN & R. S. JULIUS	428
Error Bounds in Gaussian Integration of Functions of Low-Order Con- tinuity	PHILIP RABINOWITZ	431
An Explicit Sixth-Order Runge-Kutta Formula	H. A. LUTHER	434
A Note on a Maximum Principle for the DuFort-Frankel Difference Equation	PAUL GORDON	437
The Evaluation of a Class of Functions Defined by an Integral	D. B. HUNTER	440
Some Integrals of the Arctangent Function	M. L. GLASSER	445
Simplified Calculation of $Ei(x)$ for Positive Arguments, and a Short Table of $Shi(x)$	ROBERT F. TOOPER & JOHN MARK	448