

Numerical Evaluation of Multiple Integrals I

Introduction. Several specific methods for numerical evaluation of integrals over higher dimensional regions have been proposed. James Clerk-Maxwell [1] proposed the formulas for the rectangle and the rectangular parallelepipedon in 1877. Appell, Burnside, Ionescu, and Mineur have developed special formulas for planar regions. Tyler [2] recently gave formulas for rectangles, parabolic regions, cubes, and for the hypercubes. Others have developed formulas primarily for rectangular regions based on the formulas for the line.

Although the original draft of this paper antedates their results, Hammer, Marlowe and Stroud [3] have given an inductive method for numerical evaluation of integrals precise for k th degree polynomials over the n -simplex. They also show how to obtain formulas for cones based on regions for which integration formulas are given. Certain affinely symmetrical formulas for triangle and tetrahedron are given in their paper. In a sequel Hammer and Stroud [4] gave affinely symmetrical formulas precise for the quadratic and cubic polynomials over the n -simplex. W. H. Peirce [5] in his doctoral dissertation has given numerical integration formulas over the circular annulus precise for arbitrarily high degree polynomials.

Despite the variety of results and their particular interest, the theory of numerical integration in higher dimensions is in a very crude state of development in comparison with numerical integration of functions of one variable. For this reason we give here a few theorems which are actually quite simple but which evidently have escaped the awareness of most research workers. These theorems form a partial basis for development of classical type integration formulas.

The sole numerical integration device with claims to somewhat universal applicability is that called the Monte Carlo method which has been extended and popularized by S. M. Ulam and John von Neumann. Granted the presence of a suitable sequence of "random" digits or the means of generating such, the Monte Carlo methods can be applied to a large variety of problems by using high-speed digital computers. It has been stated as an advantage of Monte Carlo methods that the number of evaluation points for, say, 5 percent error does not mount as rapidly for higher dimensions as it does for classical formulas. We shall show (as Tyler, and Hammer and Stroud have shown in other cases) that the evaluation points for classical type formulas can conceivably be kept down very well. However, the problem of determining points and weights in these circumstances is a problem in the theory of equations which is difficult inherently and also because of the great variety of functions and regions of conceivable interest. In this direction the Monte Carlo method is less sensitive to the deviations among regions.

A Basic Theorem for Numerical Integration. In this section we state a theorem which greatly extends the usefulness of particular integration formulas when they are available. We limit the discussion to integration formulas of the form

$$(1) \quad \int_R w(x)f(x)dx \doteq \sum a_j f(x_j),$$

where R is an n -dimensional region in Euclidean n -space, E_n , x is a point vector in E_n , a_1, \dots, a_m are numbers (real or complex) and evaluation points x_1, \dots, x_m are in the domain of f . In particular, R will be taken as the closure of a bounded open set in E_n and the weight function $w(x)$ and f are continuous on R . That these conditions may be relaxed will not concern us. The dx indicates a volume element in E_n .

For each relevant f and a given formula (1) there is the associated error, a number $E(f)$, which we define as

$$(2) \quad E(f) = \sum a_j f(x_j) - \int_R w(x) f(x) dx.$$

Let S be another region in E_n such that there exists a transformation J with continuous nonvanishing Jacobian which maps R onto S . We write $y = Jx$ for $x \in R$. Then if $g(y)$ is defined and continuous on S we may write

$$(3) \quad \int_S w(y) g(y) dy = \int_R w(y) g(y) |J| dx,$$

where in the integrand on the right we have $y = Jx$ and $|J|$ is the absolute value of the Jacobian which may also be indicated as $\partial y / \partial x$. Now if we have an integration formula (1) for R and the choice $w(x) = w_1(y)$, then with $f(x)$ replaced in (2) by $|J|g(y)$ we have

$$(4) \quad E(|J|g) = \sum a_j |J_j| g(y_j) - \int_R w_1(y) g(y) |J| dx,$$

where $y_j = Jx_j$ and $|J_j|$ is the value of $|J|$ at x_j .

THEOREM 1. *Writing*

$$(5) \quad E(S, g) = \sum b_j g(y_j) - \int_S w_1(y) g(y) dy,$$

where $b_j = a_j |J_j|$, then $E(S, g) = E(|J|g)$ and hence from every formula of type (1) for R there is a corresponding formula of the same type for S with error functional $E(S, g)$.

COROLLARY 1.1. *If $|J|$ is constant on R then $E(S, g) = |J|E(g)$ and hence if $E(g)$ vanishes for a function g so does $E(S, g)$. In particular, if the transformation J is a nonsingular affine transformation, $|J|$ is constant.*

COROLLARY 1.2. *Identifying $w(x)$ with $w_1(y)|J|$, $y = Jx$ and $f(x)$ with $g(y)$, assuming a formula (1), gives from equation (2)*

$$(6) \quad E(S, g) = E(g) = \sum a_j g(y_j) - \int_S w_1(y) g(y) dy.$$

Theorem 1 and the two corollaries make it possible to generate integration formulas for a variety of regions. The simplest and the most important case arises

when J is an affine transformation (Corollary 1.1). Thus certain numerical integration formulas over a particular sphere precise for polynomials of at most degree k give immediately integration formulas for any ellipsoid precise for polynomials of at most degree k .

Cartesian Product Regions. Let R be the Cartesian product of two regions R_1 and R_2 in lower dimensional Euclidean spaces. Let us designate $y \in R_1, z \in R_2$ so that every $x \in R$ can be written (y, z) . Suppose there are numerical integration formulas given of type (1) for weight functions $w_1(y)$ and $w_2(z)$, defined on R_1 and R_2 respectively, so that the error functionals may be written

$$(1) \quad E(R_1, f_1) = \sum a_i f_1(y_i) - \int_{R_1} w_1(y) f_1(y) dy$$

$$(2) \quad E(R_2, f_2) = \sum b_j f_2(z_j) - \int_{R_2} w_2(z) f_2(z) dz.$$

Then we ask for a numerical integration formula over $R = R_1 \times R_2$ with weight function $w_1(y)w_2(z)$. We have, by using (1) and (2),

THEOREM 2. *Let $f(x) = f(y, z)$ be a function defined and continuous on $R = R_1 \times R_2$. Then if we define*

$$(3) \quad E(R, f) = \sum \sum a_i b_j f(y_i, z_j) - \int_{R_1} \int_{R_2} w_1(y) w_2(z) f(y, z) dy dz,$$

we have

$$\begin{aligned} E(R, f) &= \sum b_j E[R_1, f(y, z_j)] + \int_{R_1} w_1(y) E[R_2, f(y, z)] dy \\ &= \sum a_i E[R_2, f(y_i, z)] + \int_{R_2} w_2(z) E[R_1, f(y, z)] dz. \end{aligned}$$

COROLLARY 2.1. *If $f(y, z)$ is a function such that $E[R_1, f(y, z)] = 0$ for each $z \in R_2$ and $E[R_2, f(y, z)] = 0$ for each $y \in R_1$ then $E(R, f) = 0$ and the formula (3) of Theorem 2 is exact for f .*

If F_1 is a class of functions defined on R_1 , and F_2 is a class of functions defined on R_2 , then the Cartesian product class, $F = F_1 \times F_2$, of functions defined on $R_1 \times R_2$ is the class of all functions $f(y, z)$ such that $f(y, z) \in F_1$ for each $z \in R_2$ and $f(y, z) \in F_2$ for each $y \in R_1$.

COROLLARY 2.2. *If $E(R_1, f_1) = 0$ for $f_1 \in F_1$ and $E(R_2, f_2) = 0$ for $f_2 \in F_2$ then necessarily $E(R, f) = 0$ for every $f \in F_1 \times F_2$, where the error functionals are defined by (1), (2), (3). In other words, the numerical integration formula in (3) is necessarily exact for the Cartesian product of the classes of functions for which (1) and (2) are exact.*

COROLLARY 2.3. *If classes of functions F and G respectively defined on R_1 and R_2 are representable as all linear combinations of basis sets of functions f_1, \dots, f_p and g_1, \dots, g_q respectively then $F \times G$ is the set of all functions with $(f_i g_j)$ as basis.*

Proof: If $h = \sum_i \sum_j c_{ij} f_i g_j$ where the c_{ij} are constants, then $h \in F \times G$. To show that $h \in F \times G$ implies h is a linear combination of the $f_i g_j$, we observe that

$h = \sum_i a_i f_i = \sum_j b_j g_j$ where the a_i are unique functions on R_2 , and b_j are unique functions on R_1 . Let y_1, y_2, \dots, y_p be the points in R_1 such that the determinant $|f_i(y_k)|$ is not zero. Then we have with b_{jk} the value of b_j at y_k

$$\sum_i a_i f_i(y_k) = \sum_j b_{jk} g_j \quad k = 1, \dots, p$$

which are identities on R_2 . Solving for a_1, \dots, a_p we find $a_i = \sum_j c_{ij} g_j$ where c_{ij} are constants and are unique. Hence $h = \sum_i \sum_j c_{ij} f_i g_j$.

The usefulness of the Cartesian product principle is extensive. However, even here there must be limitations. Thus over the hypercube in E_n the generation of a formula based on Cartesian powers of the line segment formulas with m points gives m^n points. If n is large and $m \geq 2$, this will involve a large number of points of evaluation.

Examples. Gauss' four-point formula on the line is exact for at most 7th degree polynomials in one variable. Hence the 16-point formula

$$\sum_1^4 \sum_1^4 a_i a_j f(x_i, x_j) \doteq \iint_R f(x, y) dx dy$$

where a_i are the Gauss weights, R is the square, and x_i are the zeros of the Legendre polynomial, is exact for $f(x, y) = \sum_i \sum_j c_{ij} x^i y^j$ $0 \leq i \leq 7, 0 \leq j \leq 7$ since this class of polynomials is the Cartesian square of the class of seventh degree polynomials in one variable. Observe that this class contains all seventh degree polynomials and additional polynomials since i and j range *independently* from 0 to 7. Similarly formulas may be developed for the hypercubes.

Laguerre's 3-point formula for weight function e^{-x} , interval $0, \infty$ holds for all fifth degree polynomials. Hence

$$\sum_1^3 \sum_1^3 a_i a_j f(x_i, x_j) \doteq \int_0^\infty \int_0^\infty e^{-(x+y)} f(x, y) dx dy$$

holds exactly for every f of form $\sum_{i \leq 5} \sum_{j \leq 5} c_{ij} x^i y^j$. Thus we obtain a formula for the quadrant. A linear transformation will give a formula for an infinite planar sector. The x_i are the zeros of the Laguerre polynomials. Again these may be used to obtain formulas for octants, etc., in higher dimensions.

Combinations of Gauss formulas and Laguerre formulas give formulas for the planar half-strip, and combinations of Hermite's and Laguerre's will give formulas for the half-plane. A formula for a planar region generates a formula for the cylinder based on this region. In scattering and potential problems Cartesian product regions which are powers or products of 3-dimensional regions are common. Thus formulas for each region are useful for generating others.

P. Davis of the National Bureau of Standards wrote of an example he and P. Rabinowitz estimated and which has since been published [6]. This example is to integrate $\exp(x_1 x_2 x_3 x_4)$ over the unit cube in 4-space. We calculated an esti-

mate using the fourth "power" of the Gauss two-point formula, and obtained with these 16 points half the error reported by Davis and Rabinowitz using $2^{15} = 32,768$ points and a Monte Carlo method. Since the cost is roughly proportional to the number of points, it is seen that the classical type formula is here much more efficient. Of course this function is particularly fortunate for Cartesian power methods since it is expandable in powers of $x_1x_2x_3x_4$.

Particular Formulas for Symmetrical Regions. In a sequel to this paper we will publish a table of formulas for the regions we have considered, in detail. However, we prefer to define symmetrical regions and correspondingly symmetrical formulas in this paper and to illustrate applications in one type of case since consideration of these problems has led to a variety of solved and unsolved related ones.

Rather than introduce specialized terms we shall say a region R in n -space is *symmetrical* if: whenever it contains a point x , it also contains all points obtained from x by interchanging coordinates and changing signs of coordinates. Thus in general with a point x there are required $2^n n!$ points (including x). A *symmetrical* region R is invariant under linear transformations with matrix containing exactly one non-zero element in each row and column, that non-zero element being either $+1$ or -1 . In evaluating integrals of monomials over R , *symmetry* as defined, saves effort as indicated in the following theorem.

THEOREM 3. *The integral over a symmetrical region R of any monomial containing an odd power is zero, the integral of a product of even powers depends only on the exponents and not on their order.*

The proof of this theorem is direct in view of the supposed symmetry of R . Now if we impose a requirement of symmetry on a numerical integration formula we find that it is possible to compute useful formulas for these regions which have not heretofore been available. A numerical integration formula is *symmetrical* if the set of evaluation points is decomposable into symmetrical sets of points, each point in a symmetrical set having the same weight as the others.

THEOREM 4. *Let $\sum a_j f(x_j)$ be a symmetrical sum formula approximating the integral $\int_R f(x)dx$ for R symmetrical. In order that $\sum a_j f(x_j) - \int_R f(x)dx = 0$ for every polynomial of degree at most $2k + 1$ it is necessary and sufficient that the formula hold exactly for all monomials f of form*

$$t_1^{2k_1} \dots t_n^{2k_n}$$

where

$$k_1 \geq k_2 \dots \geq k_n \geq 0, \quad k_1 + \dots + k_n \leq k.$$

We illustrate the application of Theorem 4 by considering symmetrical regions in 3-space and indicating a method of obtaining a formula involving at most 34 points holding exactly for 7th degree polynomials. The exact formula is given for a cube. Now in 3-space an arbitrary selection of a point would involve 47 others with the same weight. Hence we select points for which the symmetry requirement does not yield as many points. In considering the problem we will use (x, y, z) as coordinates. From Theorem 4, we then solve equations only resulting from

asking that the symmetrical formula hold exactly for the following seven functions: $1, x^2, x^4, x^2y^2, x^6, x^4y^2, x^2y^2z^2$ in order to achieve a formula exact for the general seven-degree polynomial. For seventh degree in n variables with a symmetrical formula over a symmetrical region, the *same* seven functions suffice. Now let the integrals of the seven functions given over R be $I_0, I_2, I_4, I_{22}, I_6, I_{42}, I_{222}$, respectively. We choose points and weights as follows: $(x_1, 0, 0), a_1 (6)$; $(x_2, x_2, 0), a_2 (12)$; $(x_3, x_3, x_3), a_3 (8)$; $(x_4, x_4, x_4), a_4 (8)$. The integer in parenthesis indicates the number of points in the formula generated by the required symmetry if the indicated letter coordinate is not zero. Since only squares of unknown coordinates appear we let $u_1 = x_1^2, u_2 = x_2^2, u_3 = x_3^2$ and $u_4 = x_4^2$.

The equations then are:

$$\begin{aligned}
 (1) \quad & 6a_1 + 12a_2 + 8a_3 + 8a_4 = I_0 \quad f = 1 \\
 (2) \quad & 2a_1u_1 + 8a_2u_2 + 8a_3u_3 + 8a_4u_4 = I_2 \quad f = x^2 \\
 (3) \quad & 2a_1u_2^2 + 8a_2u_2^2 + 8a_3u_3^2 + 8a_4u_4^2 = I_4 \quad f = x^4 \\
 (4) \quad & 4a_2u_2^2 + 8a_3u_3^2 + 8a_4u_4^2 = I_{22} \quad f = x^2y^2 \\
 (5) \quad & 2a_1u_1^3 + 8a_2u_2^3 + 8a_3u_3^3 + 8a_4u_4^3 = I_6 \quad f = x^6 \\
 (6) \quad & 4a_2u_2^3 + 8a_3u_3^3 + 8a_4u_4^3 = I_{42} \quad f = x^4y^2 \\
 (7) \quad & 8a_3u_3^3 + 8a_4u_4^3 = I_{222} \quad f = x^2y^2z^2.
 \end{aligned}$$

It will be observed that the set constitutes seven equations in eight unknowns so that we may hope for one free choice of another equation. To indicate the solution of the equation we now form (6)-(7) and (5)-2(6) + (7) to get, respectively,

$$(8) \quad 4a_2u_2^3 = I_{42} - I_{222}$$

$$(9) \quad 2a_1u_1^3 = I_6 - 2I_{42} + I_{222}.$$

Hence if a solution to the equation system exists and the numbers on the right of (8) and (9) are not zero then neither u_1 nor u_2 is zero and hence

$$(10) \quad 4a_2 = (I_{42} - I_{222})/u_2^3$$

$$(11) \quad 2a_1 = (I_6 - 2I_{42} + I_{222})/u_1^3.$$

Now from (3)-(4) we find

$$(12) \quad 2a_1u_1^2 + 4a_2u_2^2 = I_4 - I_{22},$$

and on substituting from (10) and (11) in (12) we have

$$(13) \quad \frac{I_6 - 2I_{42} + I_{222}}{u_1} + \frac{I_{42} - I_{222}}{u_2} = I_4 - I_{22}.$$

At this point we find it expedient to assume a relationship between u_1 and u_2 , for example $u_1 = \lambda u_2$. For the cube, later on this λ shall be taken equal to unity.

For a specified λ we may solve (13) and $u_1 = \lambda u_2$ for u_2 and u_1 , and then by (10) and (11) determine a_1 and a_2 . Hence from this point we assume a_1, a_2, u_1, u_2 , as known, and proceed to find u_3, u_4, a_3, a_4 . To this end we rewrite equations (1), (2), (4), and (7) as

$$\begin{aligned}
 (1') \quad & 8a_3 + 8a_4 = I_0 - 6a_1 - 12a_2 = p_0 \\
 (2') \quad & 8a_3u_3 + 8a_4u_4 = I_2 - 2a_1u_1 - 8a_2u_2 = p_1 \\
 (4') \quad & 8a_3u_3^2 + 8a_4u_4^2 = I_{22} - 4a_2u_2^2 = p_2 \\
 (7') \quad & 8a_3u_3^3 + 8a_4u_4^3 = I_{222} = p_3.
 \end{aligned}$$

Now if there is a solution to these equations then there exists a quadratic function $z^2 + c_1z + c_0$ such that u_3 and u_4 are zeros of the function. Then, however, c_1 and c_0 must satisfy

$$\begin{aligned}
 (14) \quad & p_0c_0 + p_1c_1 + p_2 = 0 \\
 & p_1c_0 + p_2c_1 + p_3 = 0.
 \end{aligned}$$

Assuming such a solution c_0 and c_1 we find u_3 and u_4

$$(15) \quad u_3 = \frac{-c_1 - \sqrt{c_1^2 - 4c_0}}{2}, \quad u_4 = \frac{-c_1 + \sqrt{c_1^2 - 4c_0}}{2},$$

and by substitution in (1') and (2') we may then find a_3 and a_4 . It is not simple to prove that (14) is solvable, nor that u_3 and u_4 are positive as determined. It is quite conceivable that symmetrical regions exist for which some of these wishes are not fulfilled.

We now let R be the cube of edge 2, center (0, 0, 0) and with edges parallel to the axes. Then $I_0 = 8, I_2 = 8/3, I_4 = 8/5, I_{22} = 8/9, I_6 = 8/7, I_{42} = 8/15, I_{222} = 8/27$ and we find the following solution if we let $\lambda = 1$, i.e., $u_1 = u_2$,

$$\begin{aligned}
 a_1 &= \frac{1078}{3645} & x_1 &= \sqrt{\frac{6}{7}} \\
 a_2 &= \frac{343}{3645} & x_2 &= x_1 = \sqrt{\frac{6}{7}} \\
 u_3 &= \frac{960 - 3\sqrt{28,798}}{2726} & u_4 &= \frac{960 + 3\sqrt{28,798}}{2726} \\
 x_3 &= \sqrt{u_3} & a_3 &= \frac{230 - 774u_3}{1215(u_4 - u_3)} \\
 x_4 &= \sqrt{u_4} & a_4 &= \frac{774u_4 - 230}{1215(u_4 - u_3)}.
 \end{aligned}$$

The evaluation points all lie in the cube and the weights are positive, both features being desirable for many applications. It is possible to solve the system

with other specializations. In case one takes $u_4 = 0$ then two 27-point formulas evolve, but some of the points of each lie outside the cube as James Clerk-Maxwell found in 1877. The 27-point formulas for the sphere will be given in the sequel. These too, have points outside the sphere.

Let us consider an interpretation of the 34-point formula given here for the cube. Let f be a function and let the formula be applied to approximate the integral over R . If one takes any seventh degree polynomial function agreeing with f at the 34 evaluation points, it will have the integral given by the formula no matter how the remaining $120 - 34 = 86$ degrees of freedom are used to determine the particular 7th degree polynomial since there are 120 terms in the general 7th degree polynomial. These 86 degrees of freedom are available to achieve better error estimates (but not, of course, a smaller error). The formula may be used as a formula for the parallelepipedon by Corollary 1.1.

Error Analysis. In general, error analysis in higher dimensions is much more difficult than for the function of one variable. Nevertheless, it is perhaps of value to summarize briefly one type of error analysis. Let

$$E(f) = \sum a_j f(x_j) - \int_R w(x) f(x) dx.$$

Let P be a class of functions p such that $E(p) = 0$. Then P may be considered as a linear space since if $p_1 \in P$ and $p_2 \in P$ then $E(c_1 p_1 + c_2 p_2) = 0$. Now for any particular f chose $p \in P$ and define r by $f - p = r$. Then

$$E(f) = E(p + r) = E(r) = \sum a_j r(x_j) - \int_R w(x) r(x) dx.$$

This statement holds for all $p \in P$ and every appropriate f .

We want to choose p for a given f so that there is a calculable bound to $|E(r)|$ and hence to $|E(f)|$. First choose p so that $p(x_j) = f(x_j)$. Then $r(x) = 0$ and $E(r) = - \int_R w(x) r(x) dx$ so that $|E(r)| \leq b \int_R w(x) dx$ if $|r(x)| \leq b$. The associated approximation problem is to find $p \in P$ so that $p(x_j) = f(x_j)$ and so that $\max |f - p|$ is minimized. If this can be done, we have achieved the best error bound associated with the last inequality. On the other hand, if one takes $p \in P$ such that $\max |f(x) - p(x)| \leq b$ for x ranging over R and any x outside R and if

$$a_j \geq 0, \quad \sum a_j = \int_R w(x) dx,$$

then

$$|E(f)| \leq 2b \int_R w(x) dx.$$

In applications the class P does not contain all the functions p such that $E(p) = 0$ since these are unknown and essentially unknowable.

Example. Hammer has devised a code for IBM 650 use which has been checked out by Gerald Bartholomew. This code is capable of numerical integration over any symmetrical region in E_3 using 34, 27, 14, 8, or 6 points. For a test calculation

the integral of $1/\sqrt{x} + 1/\sqrt{y} + 1/\sqrt{z}$, was approximated over the cube with center $(1/2, 1/2, 1/2)$ and edge 1. The 34-point formula here described was used and the result was 6.04 compared to the exact value 6.

Conclusion. We have here summarized a few of the useful theorems for generating numerical integration formulas from given ones, and illustrated one particular approach to obtaining formulas for symmetrical regions. In a sequel we will present all the particular formulas we have calculated for symmetrical regions including some for circle, square, sphere, cube, hypersphere, and hypercube. The method of attack presented for symmetrical regions does not hold much promise of effective extension to arbitrarily high-degree polynomials such as Peirce has carried out for the circular annulus. However, variations and extensions of these methods will be forthcoming.

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Solution of Poisson's Equation by Relaxation Method—Normal Gradient Specified on Curved Boundaries

Introduction. In the application of the relaxation technique to the solution of the Poisson's equation when the normal gradient of the wanted function, w , is specified along a curved boundary, difficulty has been experienced in finding a suitable finite difference approximation to the Poisson's equation at nodes that lie adjacent to the curved boundary. It is proposed to present in this article results which will be found adequate for tackling any type of curved boundary in two dimensions.

This problem was treated by R. V. Southwell by means of the membrane analogy developed by him [1]. It is, however, preferable to base the approximate representation of differential equations on finite difference theory, which indicates the order of the error involved in the approximation. This has been fully achieved in the case of the Poisson's equation when the boundary condition consists in