NUMERICAL INTEGRATION OF FUNCTIONS OF SEVERAL VARIABLES

G. W. TYLER

1. Introduction. Methods of mechanical quadrature of functions of more than one variable apparently have received little systematic investigation and the few available results are widely scattered in the literature. In this paper a systematic approach to this problem is given and a number of formulae are derived which may prove to be useful.

It seems worthwhile to distinguish between two types of situations in which numerical integration may be employed advantageously. When the function to be integrated is defined analytically, its value at any point may be calculated to any desired accuracy and, in such instances, one can use methods of great strength (in the sense of high polynomial accuracy) at the cost of computing accurately a comparatively small number of values of the function, at points which may often be awkwardly located. Gauss's formula for integrating functions of one variable is an example of this sort. On the other hand, when the function is defined empirically and the values must be measured rather than calculated, the accurate location of points at which values are taken may become difficult and less meaningful and the observed values themselves may be subject to a substantial error of measurement. Circumstances of this sort call for a formula which is based on easily located points and which is as unresponsive to errors of measurement as can be arranged, even though its strength may fall somewhat below the greatest obtainable. Formulae of both kinds are developed in this paper. Since the approach employed here has been used in devising integration formulae for single integrals [**12**] it may be helpful to outline briefly the development of some of them.

2. Single integrals. With proper choice of origin and scale, a definite integral over any finite range may be written in the form

$$I = \int_0^1 f(x)\,dx. \tag{1}$$

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This paper in part summarizes a more detailed unpublished study, ***The Experimental Evaluation of Definite Integrals***, which was done largely while the writer was a member of the Scientific Staff of the U.S. Navy Electronics Laboratory, and accepted as a doctoral dissertation by Virginia Polytechnic Institute in 1949. Dr. D. B. DeLury offered helpful suggestions in the preparation of this paper, and the figures were drawn by Mr. C. J. VanVliet of the U.S. Navy Electronics Laboratory. The writer is presently an Operations Analyst at Headquarters, U.S. Air Force.

It is assumed that $f(x)$ is, or may be replaced by, a polynomial of degree n,

$$(2) \qquad f(x) = \sum_{i=0}^{n} A_i x^i.$$

With this assumption

$$(3) \qquad I = \sum_{i=0}^{n} \frac{A_i}{i+1}.$$

Let an approximation to I be given by

$$(4) \qquad I_1 = \sum_{\alpha=0}^{m} R_\alpha y_\alpha \qquad (m \leqslant n),$$

where the R's are constants (weights) to be determined and the $y_\alpha = f(x_\alpha)$ are calculated or observed values of the function.

The difference,

$$(5) \qquad E = I_1 - I,$$

will be called the polynomial error.

Expanding the right side of (5) and equating to zero the coefficients of the A's, we are led to the system of equations

$$(6) \qquad \sum_{\alpha=0}^{m} R_\alpha x_\alpha{}^i = \frac{1}{i+1} \qquad (i = 0, 1, \ldots, n).$$

When the x values are chosen equally spaced over the interval of integration, including the end points, and $m = n$, the system of equations (6) leads directly to the Newton-Cotes integration formula. The values of the R_α determined by the equations are the Cotes numbers.

Clearly the arbitrary assignment of abscissa values always leads to a problem of the same type, whose solution depends on a system of linear equations.

When the x values are not chosen arbitrarily but are selected to satisfy as many as possible of the set of equations (6), and perhaps other conditions as well, the equations are no longer linear and the solutions are more difficult to obtain. Some slight simplification may be accomplished by noticing that if a set of values x_α ($\alpha = 0, 1, \ldots, m$) is a solution of (6), so also is the set $(1 - x_\alpha)$. To take advantage of this symmetry, we can write

$$(7) \qquad I = \int_{-1}^{1} F(x)\,dx = 2\int_0^1 Q(x)\,dx,$$

where $Q(x)$ is the even part of $F(x)$. Placing

$$I_1 = \sum_{\alpha=0}^{m} R_\alpha[F(x_\alpha) + F(-x_\alpha)]$$

and proceeding as before, we obtain the set of equations, analogous to (6),

$$\sum_{\alpha=0}^{m} R_\alpha x_\alpha^{\,2i} = \frac{1}{2i+1} \qquad (i = 0, 1, \ldots, n). \tag{8}$$

If we determine the R_α and x_α so that the first $2m + 2$ equations of (8) are satisfied, we obtain the Gauss formula, which has the highest possible polynomial accuracy. Some indication of the circumstances in which this formula might be deemed inappropriate is provided by the opinion of Gauss, who wrote that the x values should always be expressed in sixteen decimals to insure no error in the first $2m$ terms of (7). It is doubtful, therefore, that a formula of this kind would be useful with experimental data.

Errors in the experimental determination of $F(x_\alpha)$ would usually be expected, even if the x_α could be located without error. Often it is reasonable to assume that these errors are independent and have constant variance. It then follows easily that a formula with equal weights is the least responsive to these errors. Tchebichef's formulae were constructed to satisfy this condition and in applications, as with the Gauss formulae, it is necessary to determine function values at points that must be located with high accuracy.

3. The integral over a rectangle of a function of two variables. The integral to be evaluated will be written

$$I = \int_{-a}^{a} \int_{-b}^{b} F(x, y)\, dx\, dy, \tag{9}$$

and it will be assumed that

$$F(x, y) = \sum_{i=0}^{2n} \sum_{j=0}^{2n} A_{ij} x^i y^j, \qquad i + j \leqslant 2n. \tag{10}$$

Let

$$I_1 = 4ab \sum_{\alpha=1}^{m} R_\alpha F(x_\alpha, y_\alpha). \tag{11}$$

Substitution of the polynomial form of $F(x, y)$ in both I and I_1 yields the relation

$$\begin{aligned} I_1 - I = 4ab\Bigg[& A_{00}\left(\sum_{\alpha=1}^{m} R_\alpha - 1\right) + A_{10}\left(\sum_{\alpha=1}^{m} R_\alpha x_\alpha\right) + \ldots \\ & + A_{2i,2j}\left(\sum_{\alpha=1}^{m} R_\alpha x_\alpha^{\,2i} y_\alpha^{\,2j} - \frac{a^{2i} b^{2j}}{(2i+1)(2j+1)}\right) + \ldots \\ & + A_{0,2n}\left(\sum_{\alpha=1}^{m} R_\alpha y_\alpha^{\,2n} - \frac{b^{2n}}{2n+1}\right)\Bigg]. \end{aligned} \tag{12}$$

Equating to zero the coefficients of A_{ij} we are led to the system of equations

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$$\sum_{\alpha=1}^{m} R_\alpha x_\alpha^{\,i} y_\alpha^{\,j} = \frac{a^i b^j}{(i+1)(j+1)}, \qquad i, j \text{ both even,} \tag{13}$$
$$= 0, \qquad \text{otherwise.}$$

The problem of devising integration formulae thus becomes the problem of finding solutions to sets of equations drawn from (13). For example, for $m = 4$, a solution of the first three equations yields the obvious rule, analogous to the trapezoidal rule:

$$\int_{-a}^{a} \int_{-b}^{b} F(x,y)\,dx\,dy = ab[F(a,b) + F(a,-b) + F(-a,b) + F(-a,-b)]. \tag{14}$$

This rule is exact when $F(x, y)$ is linear. If $F(x, y)$ is a polynomial of degree 2 or 3, the error committed is easily calculated to be

$$I_1 - I = E' = \tfrac{8}{3}ab(A_{20}a^2 + A_{02}b^2). \tag{15}$$

Even if $F(x, y)$ is not of degree 3, the magnitude of the error introduced by those terms of degree one higher than that for which a formula is exact may occassionally be useful in selecting an appropriate formula. A value of E', defined in this manner, is therefore attached to each integration formula.

When $m = 5$, the first ten equations of (13) can be satisfied by the following values:

$$\begin{array}{lllll} R_1 = \frac{1}{6}, & R_2 = \frac{1}{6}, & R_3 = \frac{1}{6}, & R_4 = \frac{1}{6}, & R_5 = \frac{1}{3}, \\ x_1 = a, & x_2 = 0, & x_3 = -a, & x_4 = 0, & x_5 = 0, \\ y_1 = 0, & y_2 = b, & y_3 = 0, & y_4 = -b, & y_5 = 0. \end{array}$$

The resulting formula will be called the first five-point third degree accuracy formula:

$$\int_{-a}^{a} \int_{-b}^{b} F(x,y)\,dx\,dy = \tfrac{2}{3}ab[2F(0,0) + F(a,0) + F(-a,0) + F(0,b) + F(0,-b)], \tag{16}$$
$$E' = \tfrac{4}{45}ab(6A_{40}a^4 - 5A_{22}a^2b^2 + 6A_{04}b^4).$$

Another set of solutions to the same equations, obtained by taking points at the centre and corners of the rectangle, yields the second five-point third degree accuracy formula:

$$\int_{-a}^{a} \int_{-b}^{b} F(x,y)\,dx\,dy = \tfrac{1}{3}ab[8F(0,0) + F(a,b) + F(a,-b) + F(-a,b) + F(-a,-b)], \tag{17}$$
$$E' = \tfrac{8}{45}ab(3A_{40}a^4 + 5A_{22}a^2b^2 + 3A_{04}b^4).$$

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If an area of integration can be broken down into a number of rectangles of equal dimensions, the first five-point formula can be applied to each rectangle and the results added, to furnish a simple rule, similar in nature to Simpson's rule. Each interior point will have a weight of 2, either because it is at the centre of a rectangle or because it is on the boundaries of two rectangles, while each point on the perimeter of the area will have unit weight. Thus, if there are p perimeter points and q interior points the integral over the total area is given by

$$\iint F(x, y)\, dx\, dy = \frac{\text{total area of rectangles}}{p + 2q} [\Sigma(\text{function values at perimeter points}) + 2\Sigma(\text{function values at interior points})]. \tag{18}$$

This rule gives near equal weighting to the function values which may, in some applications, be desirable.

The second five-point formula, similarly used, leads to another formula of the same kind. The details need not be given here.

A continuation of this approach to obtain formulae of higher polynomial accuracy becomes tedious. Some simplicity may be gained by taking advantage of symmetry. For a fifth degree function,

$$I = 4ab(A_{00} + \tfrac{1}{3}A_{20}a^2 + \tfrac{1}{3}A_{02}b^2 + \tfrac{1}{5}A_{40}a^4 + \tfrac{1}{9}A_{22}a^2b^2 + \tfrac{1}{5}A_{04}b^4).$$

which may be written as

$$I = \tfrac{4}{45}ab(45M + 15N + 9P + 5Q) \tag{19}$$

$$M = A_{00},\ N = A_{20}a^2 + A_{02}b^2,\ P = A_{40}a^4 + A_{04}b^4,\ Q = A_{22}a^2b^2.$$

We wish to find values of $F(x, y)$, at a number of symmetrically and conveniently located points, which properly weighted and summed, will be equal to the value of the integral. If we choose the centre of the rectangle, $(0, 0)$, the centres of the four sides, $(0 \pm b)$ and $(\pm a, 0)$, and the four corners, $(\pm a, \pm b)$, a direct calculation shows that $F(0, 0) = M$, the sum of the values at the centres of the sides is $4M + 2N + 2P$ and the sum of the values at the four corners is $4(M + N + P + Q)$. If these three sets, properly weighted, are to furnish a value for the integral, we must have identically in M, N, P, Q,

$$45M + 15N + 9P + 5Q \equiv \alpha M + \beta(4M + 2N + 2P) + 4\gamma(M + N + P + Q). \tag{20}$$

Hence

$$\begin{aligned} \alpha + 4\beta + 4\gamma &= 45, \\ 2\beta + 4\gamma &= 15, \\ 2\beta + 4\gamma &= 9, \\ 4\gamma &= 5. \end{aligned}$$

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Since this set of equations is inconsistent, it is impossible to obtain fifth degree accuracy using this set of nine points or, apparently, any other similarly selected set of nine points.

If, in addition to the nine points considered above, we take the four points midway from the centre to the midpoints of the sides, a solution is obtained. The sum of the function values at these four points is $4M + \frac{1}{2}N + \frac{1}{8}P$ which, given a weight δ and added to the right side of (20), produces a consistent set of equations

$$\begin{aligned} \alpha + 4\beta + 4\gamma + 4\delta &= 45, \\ 2\beta + 4\gamma + \tfrac{1}{2}\delta &= 15, \\ 2\beta + 4\gamma + \tfrac{1}{8}\delta &= 9, \\ 4\gamma \qquad &= 5. \end{aligned}$$

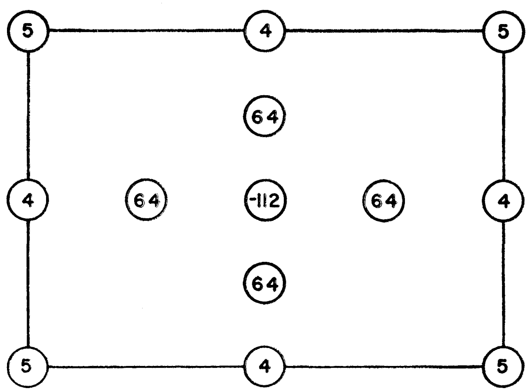
The solutions are

$$\alpha = -28, \quad \beta = 1, \quad \gamma = 5/4, \quad \delta = 16.$$

The positions of the points and the corresponding weights are shown in Figure 1, following a scheme used by Bickley [**2**]. It is easily verified that the solutions obtained here satisfy the first twenty-one equations of (13) with $m = 13$.

FIGURE 1

Thirteen-Point Fifth Degree Accuracy Formula for Double Integrals



$$\int_{-a}^{a}\int_{-b}^{b} F(x,y)\,dx\,dy = \tfrac{1}{45}ab\Big[-112F_1 + 4\sum F_2 + 5\sum F_3 + 64\sum F_4\Big] \tag{21}$$

where

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$$F_1 = F(0, 0)$$

$$\sum F_2 = F(0, b) + F(a, 0) + F(0, -b) + F(-a, 0)$$

$$\sum F_3 = F(a, b) + F(a, -b) + F(-a, b) + F(-a, -b)$$

$$\sum F_4 = F(0, \tfrac{1}{2}b) + F(\tfrac{1}{2}a, 0) + F(0, -\tfrac{1}{2}b) + F(-\tfrac{1}{2}a, 0)$$

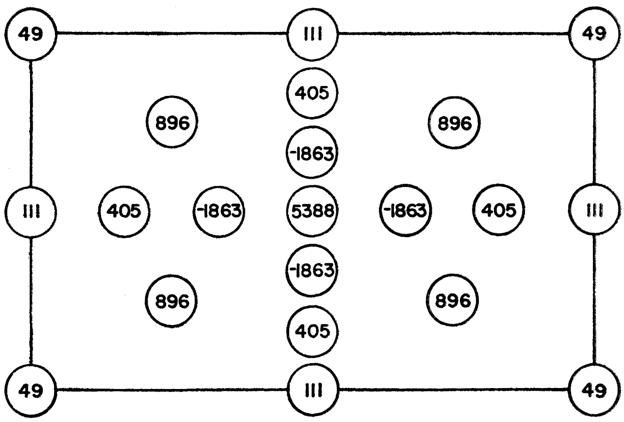
and

$$E' = \tfrac{2}{21}\, ab(A_{60}\, a^6 + A_{06}\, b^6) + \tfrac{8}{45}\, ab(A_{42}\, a^4 b^2 + A_{24}\, a^2 b^4).$$

The approach used in reaching the thirteen-point formula, (21), may be continued without alteration to establish the following twenty-one-point, seventh degree accuracy formula.

FIGURE 2

Twenty-One-Point Seventh Degree Accuracy Formula for Double Integrals



$$(22) \quad \int_{-a}^{a} \int_{-b}^{b} F(x, y)\, dx\, dy = \tfrac{1}{945}\, ab \Big[5388 F_1 + 111 \sum F_2 + 49 \sum F_3 + 405 \sum F_4 + 896 \sum F_5 - 1863 \sum F_6 \Big]$$

where $F_1 = F(0, 0)$

$$\sum F_2 = F(0, b) + F(a, 0) + F(0, -b) + F(-a, 0)$$

$$\sum F_3 = F(a, b) + F(a, -b) + F(-a, -b) + F(-a, b)$$

$$\sum F_4 = F(0, \tfrac{2}{3}b) + F(\tfrac{2}{3}a, 0) + F(0, -\tfrac{2}{3}b) + F(-\tfrac{2}{3}a, 0)$$

$$\sum F_5 = F(\tfrac{1}{2}a, \tfrac{1}{2}b) + F(\tfrac{1}{2}a, -\tfrac{1}{2}b) + F(-\tfrac{1}{2}a, -\tfrac{1}{2}b) + F(-\tfrac{1}{2}a, \tfrac{1}{2}b)$$

$$\sum F_6 = F(0, \tfrac{1}{3}b) + F(\tfrac{1}{3}a, 0) + F(0, -\tfrac{1}{3}b) + F(-\tfrac{1}{3}a, 0)$$

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and

$$E' = \tfrac{1162}{25515}ab(A_{80}a^8 + A_{08}b^8) + \tfrac{2}{63}ab(A_{62}a^6b^2 + A_{26}a^2b^6) + \tfrac{14}{225}ab\,A_{44}a^4b^4.$$

If sets of symmetrically located points are used, with all members of a set retaining the same weight, some further simplification can be had by introducing the function

$$\Phi(x, y) = \tfrac{1}{4}[F(x, y) + F(x, -y) + F(-x, y) + F(-x, -y)]$$
$$= A_{00} + A_{20}x^2 + A_{02}y^2 + \ldots + A_{2i,2j}x^{2i}y^{2j} + \ldots.$$

Then

$$\int_{-a}^{a}\int_{-b}^{b} F(x, y)\,dx\,dy = 4\int_{0}^{a}\int_{0}^{b}\Phi(x, y)\,dx\,dy.$$

The adoption of $\phi(x, y)$ leads to the system of equations

$$\sum_{\alpha=1}^{m} R_\alpha x_\alpha^{2i} y_\alpha^{2j} = \frac{a^{2i}b^{2j}}{(2i+1)(2j+1)}, \tag{23}$$

for all i, j for which $i + j \leqslant 2n$. For $m = 1$,

$$R_1 = 1, \quad x_1^2 = \tfrac{1}{3}a^2, \quad y_1^2 = \tfrac{1}{3}b^2.$$

Thus we have the following four-point, third degree accuracy formula:

$$\int_{-a}^{a}\int_{-b}^{b} F(x, y)\,dx\,dy = ab[F(a/\sqrt{3}, b/\sqrt{3}) + F(a/\sqrt{3}, -b/\sqrt{3}) + F(-a/\sqrt{3}, b/\sqrt{3}) + F(-a/\sqrt{3}, -b/\sqrt{3})] \tag{24}$$

and

$$E' = \tfrac{16}{45}ab(A_{40}a^4 + A_{04}b^4).$$

This formula, which has the same polynomial accuracy as the five-point formulae developed earlier, has the merit that all function values are weighted equally. A formula constructed from this one by adding over a set of elemental rectangles would also have this property.

For $m = 2$ there is no solution to the first six equations of (23). It is therefore impossible to obtain fifth degree accuracy using two sets of four points symmetrically disposed in this manner.

If we put $m = 3$, $x_3 = 0$, $y_2 = 0$, we obtain the equations:

$$
\begin{aligned}
&R_1 + R_2 + R_3 = 1,\\
&R_1x_1^2 + R_2x_2^2 = \tfrac{1}{3}a^2,\\
&R_1y_1^2 + R_3y_3^2 = \tfrac{1}{3}b^2,\\
&R_1x_1^4 + R_2x_2^4 = \tfrac{1}{5}a^4,\\
&R_1x_1^2y_1^2 = \tfrac{1}{9}a^2b^2,\\
&R_1y_1^4 + R_3y_3^4 = \tfrac{1}{5}b^4.
\end{aligned} \tag{25}
$$

The following values constitute a solution to this set:

$$
\begin{aligned}
R_1 &= \tfrac{9}{49}, & R_2 = R_3 &= \tfrac{20}{49}\\
x_1^2 &= \tfrac{7}{9}a^2 & x_2^2 &= \tfrac{7}{15}a^2\\
y_1^2 &= \tfrac{7}{9}b^2 & y_3^2 &= \tfrac{7}{15}b^2
\end{aligned}
$$

This leads to the eight-point formula (26) for fifth degree accuracy. The points and weights are shown in the following table:

α	1	2	3	4	5	6	7	8
$196R_\alpha$	9	9	9	9	40	40	40	40
x_α	$\frac{\surd 7}{3}a$	$\frac{\surd 7}{3}a$	$-\frac{\surd 7}{3}a$	$-\frac{\surd 7}{3}a$	$\sqrt{\frac{7}{15}}a$	$-\sqrt{\frac{7}{15}}a$	0	0
y_α	$\frac{\surd 7}{3}b$	$-\frac{\surd 7}{3}b$	$\frac{\surd 7}{3}b$	$-\frac{\surd 7}{3}b$	0	0	$\sqrt{\frac{7}{15}}b$	$-\sqrt{\frac{7}{15}}b$

Points 5 and 6 may be interpreted as four points which have become coincident in pairs, and hence the function at each of these points would have double the weight indicated by R_α in the solution of (25). This interpretation also holds for points 7 and 8.

For (26) (see next page),

$$E' = \tfrac{16}{14175}ab[-53(A_{60}a^6 + A_{06}b^6) + 70(A_{42}a^4b^2 + A_{24}a^2b^4)].$$

The above formula, written for integrating over a square of side 2 units was given by Burnside in 1908 [3]. He gave no details of its derivation but stated that it was constructed by a procedure closely similar to that which gives Gauss's two-point third degree accuracy and three-point fifth degree accuracy formulae for single integrals. Burnside illustrated the use of his formula by approximating the value of the two integrals:

$$\text{(i)} \quad \int_0^1\int_0^1 \frac{dx\,dy}{\surd(3 - x^2 - y^2)}, \qquad \text{(ii)} \quad \int_0^1\int_0^1 \frac{dx\,dy}{\surd(2 - x^2 - y^2)}.$$

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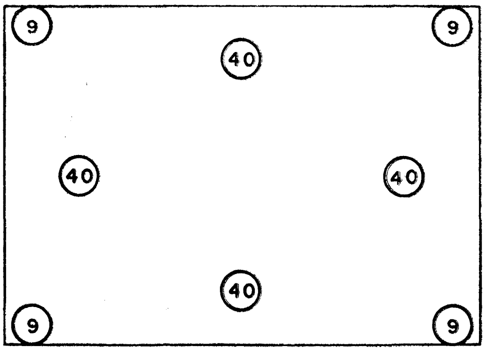
FIGURE 3

Eight-Point Fifth degree Accuracy Formula for Double Integrals



$$\text{(26)} \quad \int_{-a}^{a} \int_{-b}^{b} F(x, y)\, dx\, dy$$

$$= \tfrac{1}{49} ab[9 \sum F(\pm \tfrac{\sqrt{7}}{3} a, \pm \tfrac{\sqrt{7}}{3} b) + 40 \sum F(\pm \sqrt{\tfrac{7}{15}}\, a, 0) + 40 \sum F(0, \pm \sqrt{\tfrac{7}{15}}\, b)]$$

where it is understood the summations extend over all distinct combinations of signs.

The exact values of the integrals (i) and (ii) are

(i) $\frac{1}{2}\pi(1 - 1/\sqrt{3})$, (ii) $\pi(1 - 1/\sqrt{2})$,

which, reduced to 4-figure decimals, are

(i) 0.6639, (ii) 0.9202.

Burnside gives the values of these integrals, as calculated from the formula (26) as:

(i) 0.6641, (ii) 0.9262.

He points out that in the second integral the conditions are unfavorable for applying the approximation formula since both first partial derivatives of the radical in this integral increase without limit as the point $x = 1$, $y = 1$, is approached.

The integrals (i) and (ii) were used also by Aitken and Frewin [**1**] to obtain a rough numerical check on some of the formulae for double integrals which they developed.

If we return to (23) and put $m = 4$,

$$\frac{x_1}{a} = \frac{y_1}{b}, \quad \frac{x_2}{a} = \frac{y_2}{b}, \quad x_4 = y_3 = 0,$$

the first ten equations yield the solutions:

$$\frac{x_1}{a} = \frac{y_1}{b} = \frac{\sqrt{114 - 3\sqrt{583}}}{287} = 0.380555; \quad R_1 = \frac{178981 + 2769\sqrt{583}}{472230} = 0.520593;$$

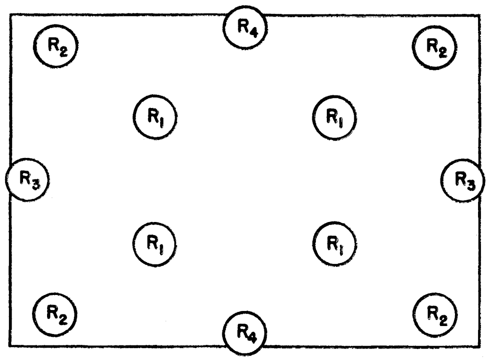
$$\frac{x_2}{a} = \frac{y_2}{b} = \frac{\sqrt{114 + 3\sqrt{583}}}{287} = 0.805980; \quad R_2 = \frac{178981 - 2769\sqrt{583}}{472230} = 0.237432;$$

$$\frac{x_3}{a} = \frac{y_4}{b} = \sqrt{\frac{6}{7}} = 0.925820; \quad R_3 = R_4 = \frac{49}{405} = 0.120988.$$

This leads to the twelve-point seventh degree accuracy formula (27).

FIGURE 4

Twelve-Point Seventh Degree Accuracy Formula for Double Integrals



$$(27) \quad \int_{-a}^{a}\int_{-b}^{b} F(x, y)\,dx\,dy = ab[R_1\sum F(\pm x_1, \pm y_1) + R_2\sum F(\pm x_2, \pm y_2) + 2R_3\sum F(\pm x_3, 0) + 2R_4\sum F(0, \pm y_4)].$$

The remainder error is:

$$E' = ab[-0.013184(A_{80}\,a^8 + A_{08}\,b^8) + 0.020441(A_{62}\,a^6b^2 + A_{26}\,a^2b^6) - 0.010035\,A_{44}\,a^4b^4].$$

For the value of the integrals which Burnside used as a rough check for his formula, the above twelve-point formula gives (i) 0.6639 and (ii) 0.9161. The approximations are seen to be better than the approximations for these integrals from Burnside's formula, though the approximation for (ii) is still in error by 4 units in the third significant figure.

4. Relative merits of the eight- and thirteen-point formulae and the twelve- and twenty-one-point formulae. If $F(x, y)$ is of the fifth degree, there are twenty-one coefficients $(A_{i,j})$. This means that there are twenty-one disposable constants, which can be used, except in special cases which we shall not discusss here, to make $F(x, y)$ pass through twenty-one points of, or satisfy a variety of other conditions with respect to, an experimentally obtained function. In statistical terms, this function has twenty-one degrees of freedom. It is evident then that the eight-point or the thirteen-point formula, with its respective number of measurements, in so far as the integration is concerned will dispose of these twenty-one degrees of freedom without error. In the problem of estimating the value of the double integral of a function taken over a single rectangle, the eight-point formula is 13/8 as efficient as the thirteen-point formula in controlling the polynomial error. If, however, we consider applying these formulae to a large number of equal-sized elemental rectangles, we see that this advantage of the eight-point formula is decreased, though apparently for all shapes of areas it will exist, at least to a small extent. The advantage of the eight-point formula decreases, of course, because the points located on the perimeter of the elemental rectangles may be coincident for two, three, or four of these rectangles. A situation favourable to the thirteen-point formula in this respect, occurs in the problem of estimating the integral over a rectangle, which, to increase the accuracy, has been subdivided into n^2 smaller rectangles similar to the original. The eight-point formula would require $8n^2$ function evaluations, compared with $8n^2 + 4n + 1$ evaluations for the thirteen-point formula. It follows that for $n = 5$ an increase of about 10 per cent in the number of function value determinations would be required to apply the thirteen-point formula, but for $n > 50$, the corresponding increase would be less than 1 per cent.

In addition to the matter discussed in the last paragraph, it is evident that application of the eight-point formula would result in weights (R_α) for each point which would be more nearly equal than the weights that would result from applying the thirteen-point formula. On the other hand, the location of the thirteen points could be described more simply and perhaps in some problems actually located with less error than will be the case with the eight points.

A very similar situation to that just discussed exists in regard to using the twelve- or twenty-one-point formulae. The twelve-point formula which disposes of the effects of thirty-six coefficients is highly efficient in controlling the polynomial error when applied to a single rectangle. One can readily envisage conditions under which it would seem advisable in the same problem to use a combination of different-sized rectangles and formulae of different degree accuracy.

5. Triple integrals over rectangular regions. Formulae for triple integrals can be developed by a natural extension of the methods used in the previous section. Let

(28) $$I = \int_{-a_1}^{a_1} \int_{-a_2}^{a_2} \int_{-a_3}^{a_3} F(x_1, x_2, x_3)\, dx_1, dx_2, dx_3.$$

Continuing as we did for double integrals we obtain the system of equations

(29) $$\sum_{\alpha=1}^{m} R_\alpha\, x_{1\alpha}{}^{i}\, x_{2\alpha}{}^{j}\, x_{3\alpha}{}^{k} = \frac{a_1{}^{i}\, a_2{}^{j}\, a_3{}^{k}}{(i+1)(j+1)(k+1)}, \quad \text{for } i, j, k \text{ all even,}$$
$$= 0, \qquad \text{for } i, \text{ or } j, \text{ or } k \text{ odd.}$$

Grouping the points in sets of 8, one in each octant, we obtain a simpler system than (29). One or both of these systems can, perhaps be employed advantageously in deriving formulae for higher degree accuracy, or formulae for other special purposes.

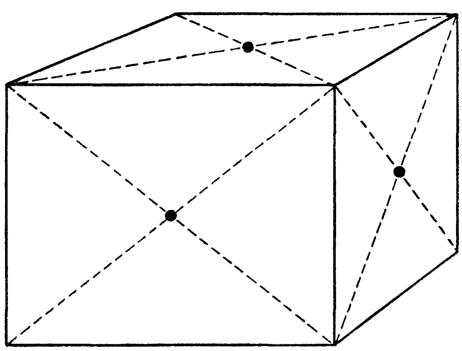
If we assume $F(x_1, x_2, x_3)$ is a third degree polynomial and integrate (28) directly we obtain:

(30) $$I = 2^3 a_1 a_2 a_3 [A_{000} + \tfrac{1}{3}\,(A_{200}\, a_1{}^2 + A_{020}\, a_2{}^2 + A_{002}\, a_3{}^2)].$$

By considering the values of $F(x_1, x_2, x_3)$ at the centre of each of the faces of the parallelepiped as shown in Figure 5, we find that the volume of the integration space multiplied by the mean of these six values is identical with (30). Hence we have the following six-point formula for third degree accuracy:

FIGURE 5

Six-Point Third Degree Accuracy Formula for Triple Integrals



(31) $$\int_{-a_1}^{a_1} \int_{-a_2}^{a_2} \int_{-a_3}^{a_3} F(x_1, x_2, x_3)\, dx_1\, dx_2\, dx_3$$
$$= \tfrac{8}{6}\, a_1\, a_2\, a_3 \Big[\sum F(\pm a_1, 0, 0) + \sum F(0, \pm a_2, 0) + \sum F(0, 0, \pm a_3) \Big],$$
$$E' = \tfrac{8}{45}\, a_1\, a_2\, a_3\, [6(A_{400}\, a_1{}^4 + A_{040}\, a_2{}^4 + A_{004}\, a_3{}^4)$$
$$- 5(A_{220}\, a_1{}^2 a_2{}^2 + A_{202}\, a_1{}^2 a_3{}^2 + A_{022}\, a_2{}^2 a_3{}^2)].$$

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In a similar manner, by considering the value of the function at the corners and centre of the parallelepiped, we obtain the following five-point formula for near third degree accuracy:

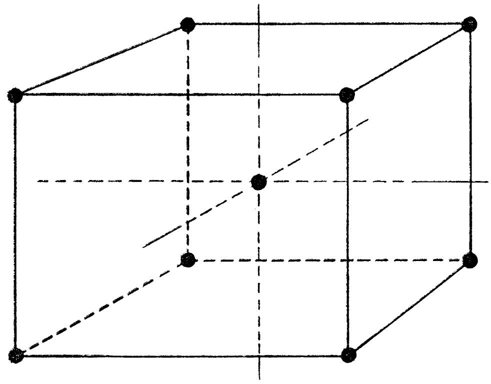
$$(32)\quad \int_{-a_1}^{a_1}\int_{-a_2}^{a_2}\int_{-a_3}^{a_3} F(x_1, x_2, x_3)\,dx_1\,dx_2\,dx_3 = \tfrac{8}{12} a_1 a_2 a_3 \,[8F(0,0,0)$$
$$+ F(a_1,a_2,a_3) + F(-a_1,a_2,-a_3) + F(a_1,-a_2,-a_3) + F(-a_1,-a_2,a_3)].$$

Using appropriate R's and coordinates as indicated by (31), it is found that the first twenty equations of (29) for $m = 6$ are satisfied. Using the R's and coordinates as shown by (32), we find that nineteen of the first twenty equations of (29) for $m = 5$ are satisfied. The only term less than fourth degree which contributes an error when using (32) is the $x_1 x_2 x_3$ term. If the coefficient A_{111} of this term is available, then subtracting $\frac{8}{3} A_{111} a_1^2 a_2^2 a_3^2$ from (32) will eliminate this error and enable us to make a full third degree precision estimate from these five points.

We can obtain a nine-point third degree accuracy formula by considering the centre and all eight vertices of the parallelepiped as shown in Figure 6. This formula is written as (33) and while it does not control the polynomial error as efficiently as either of the two preceding formulae, it gives a different coverage of the integration space and in certain problems it can be employed advantageously.

FIGURE 6

Nine-Point Third Degree Accuracy Formula for Triple Integrals



$$(33)\quad \int_{-a_1}^{a_1}\int_{-a_2}^{a_2}\int_{-a_3}^{a_3} F(x_1, x_2, x_3)\,dx_1\,dx_2\,dx_3$$
$$= \tfrac{1}{3} a_1 a_2 a_3 \left[16\, F(0, 0, 0) + \sum F(\pm a_1, \pm a_2, \pm a_3)\right],$$
$$E' = \tfrac{16}{45} a_1 a_2 a_3 \,[3(A_{400} a_1^4 + A_{040} a_2^4 + A_{004} a_3^4)$$
$$+ 5(A_{220} a_1^2 a_2^2 + A_{202} a_1^2 a_3^2 + A_{022} a_2^2 a_3^2)].$$

If we seek greater accuracy and consider the twenty-one points which as shown in Figure 7 are located at

(i) the centre of the parallelepiped,

(ii) the six midpoints of the segments joining the centre of the parallelepiped to the centre of each face,

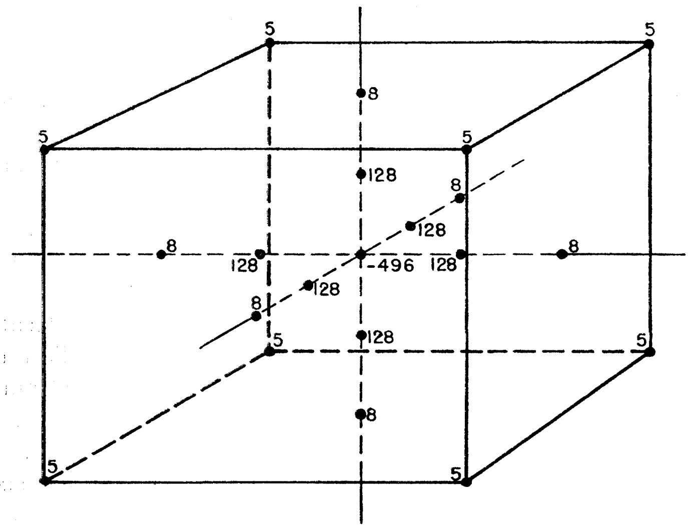
(iii) the six centres of the faces,

(iv) the eight vertices,

we obtain formula (34) which has fifth degree accuracy. The details of the derivation will be omitted but proceeding as we did in developing the thirteen-point formula (21) we can derive (34) as the result of solving only four linear equations.

FIGURE 7

Twenty-One-Point Fifth Degree Accuracy Formula for Triple Integrals



(34) $$\int_{-a_1}^{a_1}\int_{-a_2}^{a_2}\int_{-a_3}^{a_3} F(x_1, x_2, x_3)\,dx_1\,dx_2\,dx_3$$
$$= \tfrac{1}{45} a_1 a_2 a_3 \Big[-496\,F_1 + 128 \sum F_2 + 8 \sum F_3 + 5 \sum F_4 \Big]$$

where

$F_1 = F(0, 0, 0)$,

$\sum F_2$ = sum of values of the function at the 6 points located midway from the centre of the parallelepiped to the six faces,

$\sum F_3$ = sum of values of the function at the 6 centres of the faces,

$\sum F_4$ = sum of values of the function at the 8 vertices.

A feature which limits the usefulness of this formula in applications where the measurement error is heavy is the large negative weight of F_1. This can be

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improved somewhat by adjusting the position of the six points represented by $\sum F_2$, but the negative weighting cannot be eliminated in this way and it is doubtful if a more useful formula will result from such an adjustment. The general ternary quintic has 56 terms each of which might contribute an error in estimating the value of the triple integral and thus formula (34), which utilizes only twenty-one points, has high efficiency for controlling the polynomial error.

It is clear that rules can be developed, based on any one of the last four formulae, for estimating the triple integral of a function over a domain which has been subdivided into elemental parallelepipeds. In view of the equal weighting for the points and the general simplicity of (31), it appears that such a rule based on this formula would possess the greatest practical merits.

Sadowsky [**15**] developed the following 42-point formula:

$$\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\mu(x,y,z) = \tfrac{4}{225}\left[91\sum\mu_6 - 40\sum\mu_{12} + 16\sum\mu_{24}\right],$$

where $\sum\mu_6$ denotes the sum of the six values of $\mu(x, y, z)$ determined at the centres of the six faces of the cube,

$\sum\mu_{12}$ denotes the sum of the values of $\mu(x, y, z)$ at midpoints of the twelve edges of the cube,

$\sum\mu_{24}$ denotes the sum of the twenty-four values of $\mu(x, y, z)$ at the four points on the diagonals of each face and at a distance of $\frac{1}{2}\sqrt{5}$ from the centre of the face.

This formula has fifth degree accuracy and the points are all located on the surface of the cube. Sadowsky concludes that 42 is the smallest number of points that can be used to achieve this accuracy under the restraint that the points must lie on the surface. He also points out that the sixth degree function $F(x, y, z) = (x^2 - 1)(y^2 - 1)(z^2 - 1)$ vanishes at all points on the surface of the cube and hence it is impossible in general to attain as high as sixth degree accuracy under the above restraint.

6. Generalization for first degree and third degree accuracy. The possibilities of writing formulae with a given degree accuracy for any number of variables have not been explored extensively, but it is evident that some of the formulae of the preceding sections are special cases of more general formulae that can be written. Let us consider:

$$I = \int_{-a_1}^{a_1}\cdots\int_{-a_n}^{a_n} F(x_1, \ldots, x_n)\, dx_1 \ldots dx_n \tag{35}$$

where $F(x_1, \ldots, x_n)$ can be expressed in series form by

$$F(x_1, \ldots, x_n) = \sum_{\alpha_1=0}^{N}\cdots\sum_{\alpha_n=0}^{N} A_{\alpha_1\ldots\alpha_n} x_1^{\alpha_1}\ldots x_n^{\alpha_n} \tag{36}$$

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for all α_i for which

$$\sum_{i=1}^{n} \alpha_i \leqslant N.$$

If $F(x_1, \ldots, x_n)$ is linear, all the coefficients, except the first (the constant), will be neutralized in the successive integrations and we have immediately the following formula for first degree accuracy:

$$I = 2^n \prod_{i=1}^{n} a_i \, F(0, 0, \ldots, 0). \tag{37}$$

In terms of n-dimensional geometry, the almost trivial result (37) simply asserts that the integral of any linear function taken over a rectangular domain is the product of the "volume" of the integration domain and the value of the function at the centre of this domain.

If we assume $F(x_1, \ldots, x_n)$ is a third degree polynomial, then by direct integration of (35) we obtain

$$I = 2^n \prod_{i=1}^{n} a_i \, [A_{00\ldots 0} + \tfrac{1}{3} (A_{20\ldots 0}\, a_1^{\,2} + A_{02\ldots 0}\, a_2^{\,2} + \ldots + A_{00\ldots 2}\, a_n^{\,2})]. \tag{38}$$

It is evident that the expression in brackets in (38) is a weighted average of the value of the function at the centre of the integration space and at the "centres of the faces" of this space. Equation (39) gives the weighting which for all positive values of n yields (38) and is therefore a $2n + 1$ point formula with third degree accuracy for integrating over a rectangular n-space.

$$\begin{aligned} I = \frac{2^n}{6} \prod_{i=1}^{n} a_i \, [(6 - 2n)&F(0, 0, \ldots, 0) + F(a_1, 0, \ldots, 0) \\ &+ F(-a_1, 0, \ldots, 0) + F(0, a_2, \ldots 0) + \ldots + F(0, 0, \ldots, -a_n)]. \end{aligned} \tag{39}$$

7. Orthogonal polynomial methods in evaluating multiple integrals. The methods of orthogonal polynomials are useful in estimating both the observational error and the integral of functions of two or more variables. The polynomial

$$Z = f(x, y) = \sum_{\alpha=0}^{N} \sum_{\beta=0}^{N} b_{\alpha\beta} x^{\alpha} y^{\beta}, \qquad \alpha + \beta \leqslant N$$

can be rearranged and written as

$$Z = \sum_{\alpha=0}^{N} \sum_{\beta=0}^{N} B_{\alpha\beta}\, \xi_{\alpha}'(x)\, \xi_{\beta}'(y), \qquad \alpha + \beta \leqslant N \tag{40}$$

where $\xi_{\alpha}'(x)$ and $\xi_{\beta}'(y)$ are orthogonal polynomials of degree α and β in x and y respectively. In problems where the statistical error is relatively great, a realistic and effective approach is provided by fitting (40) as a regression surface to the experimental or computed values, z_{ij}. If (40) is fitted by least squares to a set of values, z_{ij}, the coefficient B_{pq} is given by

$$B_{pq} = \frac{\sum_i \sum_j z_{ij}\xi_p'(x_i)\xi_q'(y_j)}{\sum_i [\xi_p'(x_i)]^2 \sum_j [\xi_q'(y_j)]^2}. \tag{41}$$

The reduction in residual sum of squares attributable to B_{pq} is the product of B_{pq} and the numerator of this quantity as given by (41).

The arithmetic necessary for these calculations can be greatly reduced by using tabulated values of the orthogonal polynomials provided the observations are made at equally spaced x and y values. Moreover, the value of the double integral over any rectangle can be estimated by easy calculations using tabulated values for integrals of the orthogonal polynomials. The network of equally spaced observation points can either include the boundary of the integration rectangle or correspond to points at the centres of elemental rectangles within the integration rectangle.

The details of all these calculations along with an example are given by DeLury [4].

8. Double integrals over curvilinear bounded areas. In problems requiring integration over an irregularly bounded area, one can see possibilities of obtaining a more accurate and efficient approximation by the use of formulae which involve variable limits for the integrals. Though it is evident that the complexities increase rapidly as we allow the bounding surface and cylinder greater freedom, the following two formulae can be developed quite simply.

Let

$$I = \int_{-a}^{a} \int_{0}^{b(1-x^2/a^2)} F(x, y)\, dx\, dy. \tag{42}$$

Geometrically, I represents the volume under the surface $F(x, y)$ and bounded by the parabolic cylinder $y = b(1 - x^2/a^2)$ and the xy and $x\,F(x, y)$ planes. If we select the five points shown in Figure 8 and proceed in a manner closely analogous to the procedure for developing the thirteen-point rectangle formula (21), we find that we can achieve second degree accuracy for $F(x, y)$ in terms of these points.

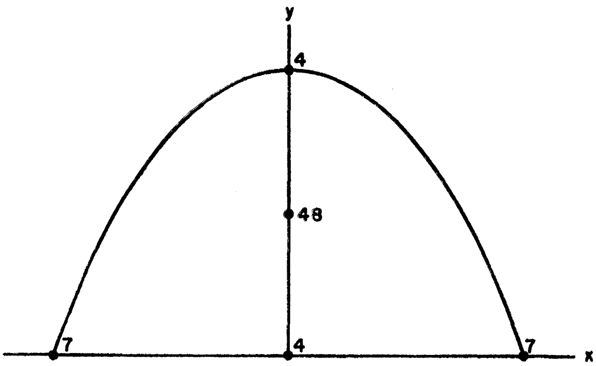
Seeking greater freedom for $F(x, y)$, we can gain simplicity by considering the doubly symmetrical integral:

$$\int_{-a}^{a} \int_{-b(1-x^2/a^2)}^{b(1-x^2/a^2)} F(x, y)\, dx\, dy. \tag{44}$$

Taking advantage of the symmetrical location of the points we can group the thirteen points shown in Figure 9 into six groups and derive, as the result of solving a set of six (we now see it could have been done with five) linear equations for the weights, the thirteen-point parabolic formula (45), which has fifth degree accuracy.

FIGURE 8

Five-Point Second Degree Accuracy Formula for Double Integrals over Parabolic Regions



$$\int_{-a}^{a}\int_{0}^{b(1-x^2/a^2)} F(x, y)\,dx\,dy = \tfrac{4}{210}\,ab\,[4F(0, 0) + 4F(0, b) + 7F(-a, 0) + 7F(a, 0) + 48F(0, \tfrac{1}{2}b)], \tag{43}$$

$$E' = -\tfrac{4}{315}\,ab\,(6A_{21}a^2b + 17A_{03}b^3).$$

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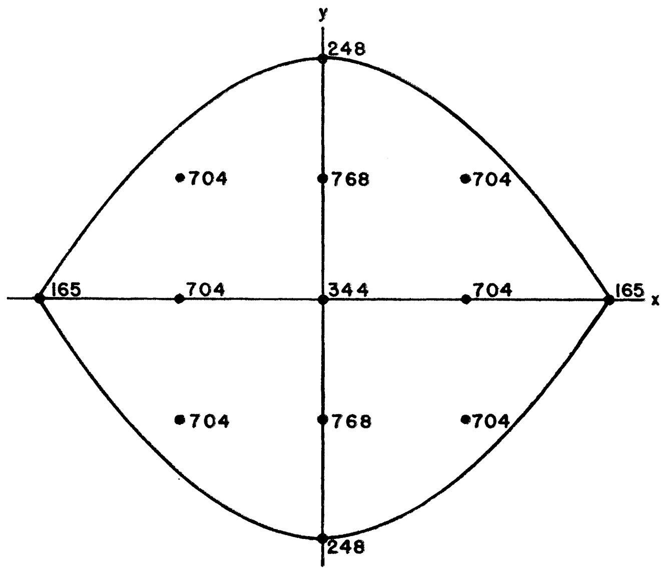
FIGURE 9

Thirteen-Point Fifth Degree Accuracy Formula for Double Integrals over Parabolic Regions



$$(45)\quad \int_{-a}^{a}\int_{-b(1-x^2/a^2)}^{b(1-x^2/a^2)} F(x,y)\,dx\,dy = \tfrac{8}{3}ab\,\tfrac{1}{6930}[344F(0,0) + 248F(0, \pm b)$$

$$+ 768F(0, \pm \tfrac{1}{2}b) + 165F(\pm a, 0) + 704F(\pm \tfrac{1}{2}a, 0) + 704F(\pm \tfrac{1}{2}a, \pm \tfrac{1}{2}b)],$$

$$E' = -\tfrac{8}{3}ab\,[\tfrac{11}{70}A_{60}a^6 + \tfrac{59}{630}(A_{42}a^4b^2 + A_{24}a^2b^4) + \tfrac{307}{2310}A_{06}b^6].$$

Attractive features of formula (45) are the simple position of the points and the near equality of weighting for all these points.

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United States Air Force
Washington 25, D.C.

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