NUMERICAL METHODS IN MULTIPLE INTEGRATION

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ABSTRACT

NUMERICAL METHODS IN MULTIPLE INTEGRATION

By

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To approximate the definite integral

$$I(f) = \int_{a_n}^{b_n} \cdots \int_{a_1}^{b_1} f(x_1, \cdots, x_n)\, dx_1 \cdots dx_n$$

over the n-rectangle,

$$R = \prod_{i=1}^{n} [a_i, b_i] ,$$

conventional multidimensional quadrature formulas employ a weighted sum of function values

$$Q(f) = \sum_{j=1}^{m} w_j f(x_{j1}, \cdots, x_{jn}).$$

Since very little is known concerning formulas which make use of partial derivative data, the objective of this investigation is to construct formulas involving not only the traditional weighted sum of function values but also partial derivative correction terms with weights of equal magnitude and alternate signs at the corners or at the midpoints of the sides of the domain of integration, R, so that when the rule is compounded or repeated, the weights cancel except on the boundary.

For a single integral, the derivative correction terms are evaluated only at the end points of the interval of integration. In higher dimensions, the situation is somewhat more complicated since as the dimension increases the boundary becomes more complex. Indeed, in higher dimensions, most of the volume of the n-rectangle lies near the boundary. This is accounted for by the construction of multi-dimensional integration formulas with boundary partial derivative correction terms, the number of which increases as the dimension increases.

Wayne Eugene Hoover

The Euler-Maclaurin Summation formula is used to obtain new integration formulas including a derivative corrected midpoint rule and a derivative corrected Romberg quadrature. Several new open formulas with Euler-Maclaurin type asymptotic expansions are presented.

The identification and utilization of the inclusion property, the persistence of form property, and the equal weight-alternate sign property coupled with the method of undetermined coefficients provide the basis for the derivation of a number of new multidimensional quadrature formulas.

These new formulas are compared with conventional rules such as Gauss' and Simpson's rules and the numerical results show the derivative corrected formulas to be more efficient and economical than conventional integration rules.

NUMERICAL METHODS IN MULTIPLE INTEGRATION

By

Wayne Eugene Hoover

A DISSERTATION

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to

my wife Diane

and

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KEY TO SYMBOLS

Symbol		Page
A	$A^{(a_1,a_1)(a_2,a_1)\cdots(a_s,a_1)(a_2,a_2)\cdots(a_s,a_s)}_{(2\beta_{11}-1,2\beta_{12}-1)(2\beta_{21}-1,2\beta_{22}-1)\cdots(2\beta_{n1}-1,2\beta_{n2}-1)}(h,k)$	54
A_c	Cubature element	97
A_m	Cubature element	97
A_0	Cubature element	97
A_c'	Cubature element	97
A_m'	Cubature element	97
A_c''	Cubature element	97
$A^{a_1 \cdots a_{s+1}}_{2\beta_1-1,\cdots,2\beta_s-1}(h)$	Quadrature formula based on the Trapezoidal rule	14
a	Lower limit of integration	7
a_i	Lower limit of integration, $i = 1(1)N$	102
$B(h)$	Boole's rule	17
$B'(h)$	DC Boole's rule	17
B_a	a-th Bernoulli number	5
$B_a(t)$	Bernoulli polynomial of degree a	5
b	Upper limit of integration	7
b_i	Upper limit of integration, $i = 1(1)N$	102
b_a	a-th modified Bernoulli number	5
$C(h)$	Midpoint rule	22
$C'(h)$	DC Midpoint rule	23
$C(h,k)$	Midpoint rule	92
$C^{2s}[a,b]$	Function space	6
$C^{2s}[R]$	Function space	38
$C^{2s,2r}[R]$	Function space	42
C^s_{0k}	DC Trapezoidal Sum	33
C^s_{mk}	$(m+1,k+1)$ entry in the DC Romberg C^s-table	34
$C^{i_1 i_2}_{j_1 j_2}$	$\lambda_{j_1 j_2}\left[a_{j_1}^{\delta_{i_1 1}} a_{j_2}^{\delta_{i_2 2}} + a_{j_2}^{\delta_{i_1 1}} a_{j_1}^{\delta_{i_2 2}}\right]$	55

Symbol		Page
c	Vector $(c_1, \cdots, c_N)$ = vertex of H or R	99
c_j	Real constant	14
c_i	i-th component of $c = \neq h_i, a_i,$ or b_i	99
$D_j(f)$	Derivative correction term, $\sum_c \sigma_j(c)\mathcal{D}_j^1 f(c)$	99
$D_{jk}(f)$	Derivative correction term, $\sum_c \sigma_{jk}(c)\mathcal{D}_j^1 \mathcal{D}_k^1 f(c)$	99
$D_j(f(v))$	Derivative correction term, $\mathcal{D}_j^1 [f(v(b_j)) - f(v(a_j))]$	104
$D_{jk}(f(v))$	Derivative correction term, $\mathcal{D}_k^1 \mathcal{D}_j^1 [f(v(a_j, a_k)) - f(v(a_j, b_k)) - f(v(b_j, a_k)) + f(v(b_j, b_k))]$	104
D_a	Derivative correction term, $f^{(a)}(b) - f^{(a)}(a)$	7
$D_{\alpha\beta}$	Partial derivative correction term	40
DC	Derivative Corrected	16
d	Dimension, number of variables	106
$d_{\alpha\beta}$	Partial derivative correction term	39
$\mathcal{D}_i^a(f)$	a-th partial derivative of f with respect to the i-th variable	96
$E(f)$	Truncation error	101
E_{2a-1}	$h^{2a}D_{2a-1}$	8
$E_{\alpha\beta}$	Partial derivative correction term	41
$F^{\alpha\beta}(t,u)$	$h^{\alpha+1}k^{\beta+1}\sum_{j=0}^{m-1}\sum_{i=0}^{n-1} f^{\alpha\beta}(x_i + th, y_j + uk)$	41
$F_h(t)$	Moving average $h\sum_{i=0}^{n-1} f(x_i + th)$	7
$F_{hk}(t,u)$	Moving average $hk\sum_{j=0}^{m-1}\sum_{i=0}^{n-1} f(x_i + th, y_j + uk)$	38
F_{ij}	$(b-a)(d-c)[h^i k^j M_{12}^{ij} + h^j k^i M_{12}^{ji}]$	111
FA	Cubature element	116
FB	Cubature element	116
FM	Cubature element	110
FO	Cubature element	110
FV	Cubature element	110
$FM1$	Cubature element	111
$FV1$	Cubature element	110
$FV11$	Cubature element	111
f	real valued function	1

Symbol		Page
$f^{(\alpha)}$	α-th derivative of f, $\mathcal{D}^\alpha f(x)$	7
$f^{\alpha\beta}$	Partial derivative of f, $\mathcal{D}_2^\beta \mathcal{D}_1^\alpha f(x,y)$	39
fe	Function evaluation(s)	13
G_i	Cubature generator	97
h	Step size, $(b-a)/n$	7
h	Hypervolume of H, $2^N h_1 \times h_2 \times \cdots \times h_N$	103
h	Hypervolume of subregion, $h_1 \times h_2 \times \cdots \times h_N$	103
h_i	Limit of integration	96
h_j	Length of subinterval, $(b_j - a_j)/\eta_j$	103
I^+	Set of positive integers	11
$I(f)$	Definite integral	
$I(f)$	$\int_a^b f(x)dx$	7
$I(f)$	$\int_c^d \int_a^b f(x,y)dxdy$	38
$I(f)$	$\int_{a_N}^{b_N} \cdots \int_{a_1}^{b_1} f(x_1, \cdots, x_N)dx_1, \cdots, dx_N$	1
$I_{\alpha\beta}$	Definite integral	40
i	index	7
i	$\sqrt{-1}$	12
j	index	38
k	Step size, $(d-c)/m$	38
$L_{\alpha\beta}$	Definite integral	41
M	Real constant	11
M_s	$\max_{a<x<b} \|f^{(s)}(x)\|$	9
$M_{\alpha\beta}$	$\max_{(x,y)\epsilon R} \|f^{\alpha\beta}(x,y)\|$	42
$M_{jk\cdots l}^{\alpha\beta\cdots\gamma}$	$\max_{x \epsilon R} \|\mathcal{D}_l^\gamma \cdots \mathcal{D}_k^\beta \mathcal{D}_j^\alpha f(x)\|$	101
m	Number of partitions of $[c, d]$	38
m	Vector $(m_1, \cdots, m_N)$	102

Symbol		Page
m_j	Midpoint, $(a_j + b_j)/2,\ j = 1(1)N$	102
N	Dimension, number of variables	96
$N(h)$	Newton Cotes' 7-point rule	17
$N'(h)$	DC Newton Cotes' 7-point rule	17
$N_{2s,a}$		42
n	Number of partitions of $[a, b]$	7
n	Number of subdivisions of R	107
n_j	Step size, $(b_j - a_j)/h_j,\ j = 1(1)d$	103
nfe	Number of function evaluations	11
$Q(f)$	Multidimensional quadrature formula	101
$Q_{a\beta}$	Partial derivative correction terms	55
$Q^{a_1 \cdots a_{s+1}}_{2\beta_1 - 1, \cdots, 2\beta_s - 1}(h)$	Quadrature formula based on the Midpoint rule	25
R	Rectangle $[a, b] \times [c, d]$	38
R	N-rectangle, $\prod_{i=1}^{N} [a_i, b_i]$	102
$R(h, a)$	Remainder integral, $F_h^a(t) B_a(t) dt$	7
$R(h, k; 2s, 2s)$	Remainder integral	41
$r(h)$	$\min_{a \in I^+} R(h, a)$	11
$S(h)$	Simpson's rule	17
$S'(h)$	DC Simpson's rule	17
$T(h)$	Trapezoidal sum, $h \sum_{i=0}^{n}{}' f(x_i)$	7
$T(h, k)$	Trapezoidal sum, $hk \sum_{j=0}^{m}{}'' \sum_{i=0}^{n}{}'' f(x_i, y_j)$	39
T_a	Trapezoidal sum, $T(ah)$	17
T_{ij}	Trapezoidal sum, $\lambda_{ij}[T(a_i h, a_j k) + T(a_j h, a_i k)]$	54
T_{0k}	Trapezoidal sum	32
T_{mk}	$(m + 1, k + 1)$ entry in Romberg T-table	32
$U(h)$	Simpson's Second rule	17
$U'(h)$	DC Simpson's Second rule	17
$u(\theta)$	$(a_1 + h_1 (i_1 - \theta), \cdots, a_N + h_N (i_N - \theta))$	103
$V(h)$	Weddle's rule	17
$V'(h)$	DC Weddle's rule	17

Symbol		Page
$v(x_j)$	$(a_1 + i_1 h_1, \cdots, x_j, a_{j+1} + i_{j+1} h_{j+1}, \cdots, a_N + i_N h_N)$	104
$v(x_j, x_k)$	$(a_1 + i_1 h_1, \cdots, x_j, a_{j+1} + i_{j+1} h_{j+1}, \cdots, x_k, a_{k+1} + i_{k+1} h_{k+1}, \cdots, a_N + i_N h_N)$	104
$w(h)$	Romberg's 9-Point rule	17
$w'(h)$	DC Romberg's 9-point rule	17
w	$w_1 \times w_2 \times \cdots \times w_N$	102
w_j	Length of j-th interval, $b_j - a_j$	102
x_i	Quadrature node, $a + ih$, $i = 0(1)n$	7
y_j	Quadrature node, $c + jk$, $j = 0(1)m$	38
α	index	6
β	index	14
γ	Positive integer	14
γ	Area of rectangle $(b - a)(d - c)$	42
$\Delta_{2\alpha-1}$	$b_{2\alpha} E_{2\alpha-1}$	8
δ_{ij}	$\begin{cases} 1 & \text{if } \beta_{ij} = 0 \\ 2\beta_{ij} & \text{otherwise} \end{cases}$	54
ϵ	is an element of	10
η	Positive integer	54
λ_{ij}	$\begin{cases} ½ & \text{if } i = j \\ 1 & \text{otherwise} \end{cases}$	54
Π	Cartesian product	1
π	Pi, 3.14159265358979 $\cdots$	12
Σ	Summation	1
$\sigma_j(c)$	$\begin{cases} -1 & \text{if } c_j = -h_j \text{ or } a_j \\ +1 & \text{otherwise} \end{cases}$	99 102
$\sigma_{jk}(c)$	$\sigma_j(c)\sigma_k(c)$	99
$\Phi(h, s)$	Derivative correction sum, $\sum_{\alpha=1}^{s} \Delta_{2\alpha-1}$	8
$\Phi(h, k; 2s, 2s)$	Partial derivative correction sum	41
$\phi_\alpha(t)$	Bernoulli polynomial of degree α	39
$\psi_\alpha(u)$	Bernoulli polynomial of degree α	39
$\Omega(h, k; 2s, 2s)$	Truncation error	56
0.74	$\pi^2/6\sqrt{5}$	42
1.48	$\pi^2/3\sqrt{5}$	42

Symbol		Page
2.17	$\pi^4/45$	6
2.66	$\pi^4/15\sqrt{6}$	9
2.95	$2\pi^2/3\sqrt{5}$	42
3.00	$3\pi^4/40\sqrt{6}$	23
5.31	$\pi^4\sqrt{6}/45$	46
5.93	$\frac{4\pi^2}{3\sqrt{5}}\left[\frac{1}{2} + \frac{\pi^2}{12\sqrt{5}} + \frac{h/12}{1-(h/2\pi)^2}\right]$	44
7.17	$\frac{4\pi^2}{3\sqrt{5}}\left[\frac{1}{2} + \frac{\pi^2}{12\sqrt{5}} + \frac{\pi}{9}\right]$	44
10.61	$2\pi^4\sqrt{6}/45$	48
11.17	$\frac{\pi^4\sqrt{6}}{45}\left[1 + 6^{-1/2} + \frac{h/6}{1-(h/2\pi)^2}\right]$	47

I. INTRODUCTION

We wish to approximate multidimensional integrals of the form

$$I(f) = \int_{a_N}^{b_N} \cdots \int_{a_1}^{b_1} f(x_1, \cdots, x_N) dx_1 \cdots dx_N \tag{1.1}$$

over the N-rectangle

$$R = \prod_{i=1}^{N} [a_i, b_i]$$

where a_i and b_i are real numbers.

The traditional methods of multidimensional numerical integration employ a weighted sum of m function values

$$Q(f) = \sum_{i=1}^{m} w_i f(x_{i1}, \cdots, x_{iN}). \tag{1.2}$$

The w_i are called weights and the $(x_{i1}, \cdots, x_{iN})$ are called nodes. The difference

$$E(f) = I(f) - Q(f) \tag{1.3}$$

is the truncation error (or error).

Let $p_k = p_k(x_1, \cdots, x_N)$ be a polynomial of degree k in N variables. We say that the multidimensional quadrature rule or formula $Q(f)$ is of order k or has degree of precision k if for any p_k, $E(p_k) = 0$, but $E(p_{k+1}) \neq 0$ for at least one polynomial p_{k+1}.

Since it is not uncommon for numerical procedures to make use of partial derivatives, e.g. in optimization techniques, it is surprising that except for work by Tanimoto [50] [1], Obreschkoff [38], and Ionescue [23], very little is known concerning the use of partial derivatives in nonproduct multidimensional quadrature rules.

[1] The numbers in brackets refer to entries in the Bibliography.

Therefore, the objective of this investigation is to construct a number of new multidimensional quadrature formulas using first- and mixed second-order partial derivatives of the integrand in addition to function values of the integrand.

It is shown that the use of partial derivatives of the integrand evaluated on the boundary of R increases both the efficiency and accuracy of composite multidimensional integration formulas.

The accuracy and efficiency are achieved by the proper combination of the following three properties.

The first is the "inclusion property". It is well known that m-point Gaussian integration rules for the N-rectangle, R, are extremely accurate. However, when R is subdivided into s subrectangles or cells and the m-point Gauss rule is applied to each cell, the total number of nodes is ms since the nodes are interior to each cell.

A more efficient procedure is to employ an integration rule in which some nodes coincide with the boundary of the domain of integration. Then when the domain is subdivided, these nodes are included in more than one cell. Thus the total number of nodes is considerably less than the sum of their numbers in each cell. We call this the "inclusion property".

The second is known as "persistence of form". Briefly, this means that for many functions, it requires approximately the same if not less computer time to evaluate the partial derivative at a point where the function is being evaluated as it does to evaluate the function at another point.

Finally, efficiency and accuracy result from applying the "equal weight-alternate sign property". Essentially this means that in the composite formulation of a rule, the weights of the partial derivative correction terms cancel at interior points and consequently, the partials need be evaluated only on the boundary of R. This results in a substantial increase in efficiency.

Numerical multiple integration is currently receiving considerable attention by numerical analysts. The first book on the subject, written by Stroud [49], appeared only recently. An excellent introduction may be found in Davis and Rabinowitz [13]. Comprehensive bibliographies are given by Fritsch [19], Stroud [49], and De Doncker and Piessens [14].

Brief surveys of the literature may be found in Ahlin [2], Hammer [21], and Hammer and Wymore [22]. A history of the Euler-Maclaurin Summation formula is given by Barnes [4].

Squire [47] devotes an entire chapter to derivative corrected quadrature formulas. Stroud [49] states only one cubature formula, C_2:2-1, which uses partial derivatives of the integrand. Lanczos [28] and Davis and Rabinowitz [13] discuss quadrature rules using derivative data. Tanimoto [50] was one of the first to consider cubature rules with partial derivative correction terms. Burnside [11] published the first nonproduct fifth-order cubature rule. Tyler [51] gave the first derivation of the 8-point Burnside formula. Finally, Price [41] gives some interesting examples.

In this dissertation, Chapter 2 provides a background for the 1-dimensional Euler-Maclaurin Summation formula (Euler [15], Maclaurin [33]). Several error estimates and an algorithm due to Frame [18] are stated.

It is shown in Chapter 3 that the Euler-Maclaurin Summation formula may be used to obtain asymptotic expansions for at least 5 of the Newton-Cotes' quadrature formulas, the midpoint formula, and several new open formulas including some with end derivative correction terms. The third-order derivative corrected midpoint rule is shown to be more efficient than the classic Simpson's rule [46]. After reviewing Romberg quadrature, we define a new technique called derivative corrected Romberg quadrature.

The 2-dimensional Euler-Maclaurin Summation formula is stated in Chapter 4. Also, several error estimates are given.

In Chapter 5, the double Euler-Maclaurin Summation formula is used to obtain asymptotic expansions for a variety of formulas. New asymptotic expansions are given for Squire's [48], Ewing's [15], Tyler's [51] and Miller's [35] rules.

The method of undetermined coefficients, the inclusion property, the persistence of form property, and the equal weight–alternate sign property are employed in Chapter 6 to construct 47 new derivative corrected cubature rules of orders 1, 3, 5, and 7. These formulas are generalizations of the midpoint, trapezoidal, Squire's [48], Ewing's [16], Tyler's [51], Miller's [35], Simpson's, and Albrecht, Collatz [3] and Meister's [34] rules. One of these, called MINTOV (for Multiple INTegration, Order 5), may be considered a generalization of Lanczos' [28] result which Lanczos calls Simpson's rule with end corrections. Error bounds are included for the 47 new cubature rules. As is shown in the case of MINTOV, these formulas may be generalized to multidimensional derivative corrected quadrature rules.

In Chapter 7, we compare the first-, third-, and fifth-order formulas of Chapter 6 with existing formulas of comparable degrees of precision. The numerical results indicate that partial derivative correction terms substantially enhance the efficiency of composite numerical integration formulas.

Conclusions and recommendations for further study are given in Chapter 8.

Lyness [29] states than an important objective of those concerned with the formulation of numerical integration techniques is "to determine which rule requires the fewest function evaluations to obtain a result of particular accuracy or degree". Thus, we will pay particular attention to minimizing the number of points at which the function or partial derivatives are to be evaluated. This will require the generalization of the equal weight-alternate sign property to higher dimensions in order to obtain efficient composite integration formulas with partial derivative correction terms. In cases where derivative information is easily obtained, we will show the superiority of the derivative corrected formulas over the traditional rules which use only function information, provided that the first- and/or mixed second-order partial derivatives are easily evaluated.

We conclude this introduction by recalling Oliver's [40] classic statement: "Now for any given formula or algorithm a pathological problem can always be devised for which an arbitrary small accuracy cannot be attained; we can therefore never argue the universality of any particular method, and we do not attempt this." Indeed, it is sufficient to take for the integrand, $f = Mp^k$, where p is a polynomial having zeros which coincide with the nodes of the integration formula, $k \geqslant 2$, and M is a sufficiently large positive constant.

2. FUNCTIONS OF ONE VARIABLE

2.1 BERNOULLI POLYNOMIALS AND NUMBERS

The Bernoulli polynomial $B_a(t)$ of degree a has the form

$$B_a(t) = \sum_{k=0}^{a} \frac{b_k t^{a-k}}{(a-k)!} \tag{2.1.1}$$

and the following properties:

$$\begin{aligned} B_0(t) &= 1 \\ B_1(t) &= t - \frac{1}{2} \\ B_{a-1}(t) &= B_a'(t) \\ B_a(1) - B_a(0) &= \sum_{k=0}^{a-1} \frac{b_k}{(a-k)!} = \begin{cases} 1 & \text{if } a = 1 \\ 0 & \text{if } a > 1. \end{cases} \end{aligned} \tag{2.1.2}$$

The last property in (2.1.2) may be used to determine the coefficients b_a. The coefficients B_a in the expansion

$$1 - \frac{x}{2} + \sum_{a=1}^{\infty} (-1)^{a-1} B_a x^{2a}/(2a)! = -\frac{x}{2} + \frac{x}{2}\coth\left(\frac{x}{2}\right) = \sum_{a=0}^{\infty} b_a x^a \tag{2.1.3}$$

are the Bernoulli numbers and are related to the b_a by the relation

$$b_{2a} = (-1)^{a-1} \frac{B_a}{(2a)!}, \quad a > 0. \tag{2.1.4}$$

It can be shown that $b_{2a+1} = 0$ for $a > 0$. Also, $b_{2a} = B_a(0) = B_a(1)$ for $a > 1$. For reference we list the first 10 Bernoulli numbers in Table 2.1.1.

Table 2.1.1 Bernoulli Numbers

a	1	2	3	4	5	6	7	8	9	10
B_a	$\frac{1}{6}$	$\frac{1}{30}$	$\frac{1}{42}$	$\frac{1}{30}$	$\frac{5}{66}$	$\frac{691}{2730}$	$\frac{7}{6}$	$\frac{3617}{510}$	$\frac{43867}{798}$	$\frac{174611}{330}$

Adams [1] lists the first 62 Bernoulli numbers. The Unpublished Math. Tables Repository has the most extensive list of Bernoulli numbers containing the first 836.

It is shown in Knopp [26] that

$$\frac{B_a(2\pi)^{2a}}{2(2a)!} = \sum_{k=1}^{\infty} \frac{1}{k^{2a}}. \tag{2.1.5}$$

This shows that the B_a increase rapidly for $a > 5$. Indeed

$$\frac{B_{a+1}}{B_a} > \frac{(a+1)(2a+1)}{2\pi^2} \longrightarrow \infty \tag{2.1.6}$$

as $a \longrightarrow \infty$.

Frame [18] gives several interesting results concerning the Bernoulli polynomials and the Bernoulli numbers.

Lemma 2.1.1

$$\int_0^1 B_a^2(t)dt = \frac{B_a}{(2a)!} \tag{2.1.7}$$

Lemma 2.1.2

$$\frac{B_a(2\pi)^{2a}}{(2a)!} \leqslant \frac{\pi^4}{45} \tag{2.1.8}$$

Comparing Lemmas 2.1.1 and 2.1.2 we see that

$$\int_0^1 B_a^2(t)dt \leqslant 2.17(2\pi)^{-2a} \tag{2.1.9}$$

where $2.17 \approx \pi^4/45$.

Lemma 2.1.3

$$|b_{4a}| \leqslant \frac{1}{2} b_{2a}^2 \tag{2.1.10}$$

Next we will state the Euler-Maclaurin Summation formula.

2.2 THE EULER-MACLAURIN SUMMATION FORMULA

Let $C^{2S}[a,b]$ be the set of all real-valued functions defined on the finite closed interval $[a,b]$ with the property that the derivatives $f^{(a)}(x)$, $a \leqslant 2s$, are continuous on $[a, b]$. Let D_a denote the following boundary derivative correction terms:

$$D_a = f^{(a)}(b) - f^{(a)}(a), a \in \mathrm{I}^+. \tag{2.2.1}$$

Partition the interval $[a,b]$ into n equal parts each of width $h = (b-a)/n$. Let the points of subdivision be denoted by $x_i = a + ih$, $i = 0(1)n$, where $x_0 = a$ and $x_n = b$.

We now define the a-th remainder integral

$$R(h,a) = \int_0^1 F_h^{(a)}(t) B_a(t) dt \tag{2.2.2}$$

in terms of the Bernoulli polynomials $B_a(t)$ and the a-th derivative of the moving average

$$F_h(t) = h \sum_{i=0}^{n-1} f(x_i + th). \tag{2.2.3}$$

The celebrated Euler-Maclaurin Summation formula expresses a sum of values of $f(x)$ evaluated at the equally spaced points x_i in terms of the definite integral

$$I(f) = \int_a^b f(x)dx \tag{2.2.4}$$

and a series consisting of constant multiples of the derivative correction terms D_{2a-1}.

Theorem 2.2.1 (Euler [15], Maclaurin [33])

For $f \in C^{2s}[a,b]$

$$\int_a^b f(x)dx = h \sum_{i=0}^{n}{}'' f(X_i) - \sum_{a=1}^{s} h^{2a} b_{2a} D_{2a-1} + \int_0^1 F^{(2s)}(t) B_{2s}(t) dt. \tag{2.2.5}$$

Here the double prime signifies that the first and last terms in the sum are assigned weights 1/2 and the remaining terms receive weights 1.

The proof of Theorem 2.2.1 follows by integrating (2.2.2) by parts and noting that

$$T(h) = h \sum_{i=0}^{n}{}'' f(x_i)$$

$$= \frac{1}{2}[F_h(0) + F_h(1)] = \mathrm{I}(f) + R(h,1), \tag{2.2.6}$$

$$\int_0^1 F_h(t)dt = \int_a^b f(x)dx, \tag{2.2.7}$$

and

$$R(h,a-1) = b_a h^a D_{a-1} - R(h,a). \tag{2.2.8}$$

Introducing the notation

$$E_{2a-1} = h^{2a} D_{2a-1} \tag{2.2.9}$$

$$\Delta_{2a-1} = b_{2a} E_{2a-1}$$

$$\Phi(h,s) = \sum_{a=1}^{s} \Delta_{2a-1},$$

we may express the Euler-Maclaurin Summation formula with remainder in the more compact form:

$$I(f) = T(h) - \Phi(h,s) + R(h,2s). \tag{2.2.10}$$

For concreteness we write the first several terms of $\Phi(h,s)$ in (2.2.10):

$$\int_a^b f(x)dx = h\sum_{i=0}^{n} f(a+ih) - \frac{h}{2}[f(a)+f(b)] - \frac{E_1}{12} + \frac{E_3}{720} - \frac{E_5}{30240} + \frac{E_7}{1209600} - \frac{E_9}{47900160} + \cdots + R(h,2s). \tag{2.2.11}$$

From this we see that the Euler-Maclaurin Summation formula is a generalization of the Trapezoidal Rule, $T(h)$. It relates a sum of equally spaced function values and an integral and states explicitly the boundary derivative correction terms which allow one to be converted into the other.

Consequently, it may be used for summation as well as for numerical quadrature. Also, it has provided the basis for some useful results in the theory of asymptotic expansions. (See Oliver [39].)

2.3 ERROR ESTIMATES

Effective application of the Euler-Maclaurin Summation formula in the approximation of sums or integrals depends on a close estimate of the remainder integral, $R(h,s)$, and a judicious selection of h and s which will achieve the required accuracy with a minimum of computational effort.

For many functions, for example rational functions, the remainder integrals $R(h,s)$ for a given h may first become smaller, but then grow without bound as s increases to infinity.

The problem is to predict the h and s which will yield the desired accuracy without compromising computational economy.

Applying the Cauchy-Schwarz inequality to (2.2.8) and applying Lemmas 2.1.1 and 2.1.2, Frame [18] obtained the following upper bounds for the quadrature error in the Euler-Maclaurin Summation formula.

Theorem 2.3.1

$$|R(h,s)| \leq 1.48(b-a)M_s\left(\frac{h}{2\pi}\right)^s, \quad s \geq 1 \tag{2.3.1}$$

where

$$M_s = \underset{a \leq x \leq b}{\text{Max}} |f^{(s)}(x)|, \tag{2.3.2}$$

$$1.48 \approx \pi^2/3\sqrt{5}.$$

For appropriate h and s, a sharper error estimate is the following.

Theorem 2.3.2

$$|R(h,2s+1)| \leq 2.66(b-a)M_{2s+2}\left(\frac{h}{2\pi}\right)^{2s+2}, \quad s \geq 1 \tag{2.3.3}$$

where 2.66 approximates $\pi^4/15\sqrt{6}$.

We observe that we now have in fact three error estimates. To see this, substitute $b_{2s+1} = 0$ in (2.2.14) to obtain

$$R(h,2s) = -R(h,2s+1). \tag{2.3.4}$$

Then using (2.3.4) in (2.3.1) we may write the estimates as follows:

$$|R(h,2s)| \leq 1.48(b-a)M_{2s}\left(\frac{h}{2\pi}\right)^{2s} \tag{2.3.5}$$

$$|R(h,2s+1)| \leq 1.48(b-a)M_{2s+1}\left(\frac{h}{2\pi}\right)^{2s+1} \tag{2.3.6}$$

$$|R(h,2s+1)| \leq 2.66(b-a)M_{2s+2}\left(\frac{h}{2\pi}\right)^{2s+2} \tag{2.3.7}$$

The selection of the appropriate estimate depends on the step size, h, the number of derivative correction terms, s, and the modulus of certain derivatives of $f(x)$ over the domain of integration.

For example, for rational integrands, the sharpest error estimate may depend on h and s as roughly indicated in Figure 2.3.1.

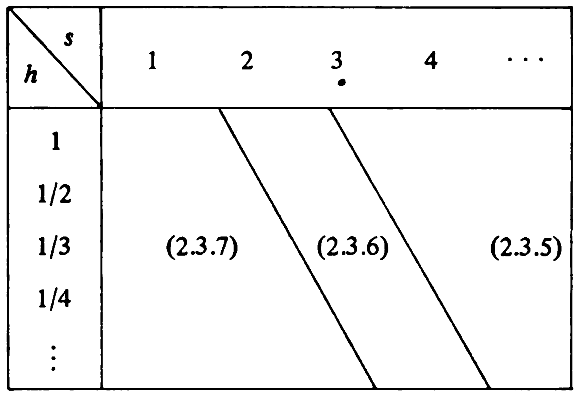

Figure 2.3.1 Values of h and s for the Best Error Estimate

Of considerable interest is the question for which functions f and for which values of h and a does $R(h,a)$ converge to zero. We are assuming $f \in C^{a}[a,b]$; hence f is Riemann integrable on $[a,b]$ and we have

$$\lim_{h \to 0} R(h,a) = 0. \qquad (2.3.8)$$

On the other hand, many functions $f \in C^{\infty}[a,b]$, e.g. rational functions, satisfy

$$\lim_{a \to \infty} R(h,a) = \infty. \qquad (2.3.9)$$

However, if we assume $f \in C^{\infty}[a,b]$ and if there are constants M and c such that

$$M_a = \max_{a < x < b} |f^{(a)}(x)| < Mc^a, \qquad (2.3.10)$$

then for $0 < h < 2\pi/c$ we have

$$\lim_{a \to \infty} R(h,a) = 0. \qquad (2.3.11)$$

Examples of functions for which (2.3.11) apply are products of functions such as exponential functions e^{kx}, trigonometric functions $\sin(kx)$, $\cos(kx)$, and Bessel functions $J_m(kx)$.

Finally, in the case $f(x) \in C^{\infty}[a,b]$ is a rational function, $f(x)$ is a sum of partial fractions of the form $a_j/(x_j - x)$ and $f^{(\alpha)}(x)$ is a sum of terms each of the form $\alpha!\, a_j/(x_j - x)^{\alpha+1}$. Moreover, there exist constants M and c such that M_α satisfies a weaker inequality

$$M_\alpha < \alpha!\, Mc^\alpha. \tag{2.3.12}$$

Therefore, for $0 < h \leq 2\pi/c$, Frame [18] has shown that

$$r(h) = \min_{\alpha \epsilon I^+} R(h,\alpha) < (b-a)M(hc)^{-1/2}10^{\left(1-\frac{30}{11\,hc}\right)} \tag{2.3.13}$$

and suggests the following algorithm for selecting a priori the step size, h, and s, the number of derivative correction terms, for use in the Euler-Maclaurin Summation formula:

(i) Given $f(x)$, a, b, and an error requirement $\varepsilon > 0$, calculate M and c according to

$$M_\alpha < \alpha!\, Mc^\alpha. \tag{2.3.14}$$

(ii) Choose h sufficiently small so that the error satisfies

$$r(h) < (b-a)M(hc)^{-1/2}10^{\left(1-\frac{30}{11\,hc}\right)} < \varepsilon. \tag{2.3.15}$$

(iii) Determine $s \,\epsilon\, I^+$ by

$$s = [\pi/hc]\,, \tag{2.3.16}$$

the greatest integer $\leq \pi/hc$.

(iv) Apply the Euler-Maclaurin Summation formula to approximate a definite integral or a sum using the above values of h and s. □

Thus, even though $\lim_{\alpha\to\infty} R(h,\alpha) = \infty$, that is, the asymptotic series diverges, it may be useful in certain applications.

The problem of a priori estimating the h and s which not only guarantee a stated error requirement but also result in maximum computational efficiency by minimizing the number of function and/or derivative evaluations (nfe) is not completely solved. It may be stated as follows.

Given $f(x) \,\epsilon\, C^\alpha[a,b]$, and $\varepsilon > 0$, find $n = (b-a)/h$ and $s \leq \alpha/2$ which minimize

$$nfe = 2s + n + 1 \tag{2.3.17}$$

subject to

$$|R(h, 2s+1)| \leq 2.66(b-a)\left(\frac{h}{2\pi}\right)^{2(s+1)} M_{2s+2} < \varepsilon. \tag{2.3.18}$$

2.4 A NUMERICAL EXAMPLE

Consider the definite integral

$$I(f) = \int_0^1 \frac{4dx}{1+x^2} = \pi. \tag{2.4.1}$$

Expand the integral into partial fractions and differentiate a times to obtain

$$f^{(a)}(x) = a!\,2i[(i-x)^{-1-a} - (-i-x)^{-1-a}]. \tag{2.4.2}$$

Since the maximum occurs at $x = 0$, we have

$$M_a < 4a! \tag{2.4.3}$$

Now set $M = 4$ and $c = 1$ in (2.3.15) to obtain

$$r(h) < 4h^{-\frac{1}{2}}10^{\left(1-\frac{30}{11h}\right)}. \tag{2.4.4}$$

Then using (2.4.4) and (2.3.16) we compute the values in Table 2.4.1.

The values of D_{2a-1} are calculated as follows.

$$\begin{aligned} D_{2a-1} &= f^{(2a-1)}(1) - f^{(2a-1)}(0) \\ &= (2a-1)!\,2^{2-a}\sin(a\pi/2). \end{aligned} \tag{2.4.5}$$

Hence, employing the Euler-Maclaurin Summation formula, we have

$$\begin{aligned} \pi &= h\sum_{i=0}^{n}{}'' \frac{4}{1+(ih)^2} \\ &\quad - \sum_{a=1}^{(s+1)/2} (-1)^a h^{4a-2} b_{4a-2}(4a-3)!\,2^{3-2a} + R(h,2s) \\ &= h\sum_{i=0}^{n}{}'' \frac{4}{1+(ih)^2} + \frac{h^2}{6} - \frac{h^6}{504} + \frac{h^{10}}{1056} - \frac{h^{14}}{384} \\ &\quad + \frac{h^{18}\,43\,867}{1\,838\,592} - \frac{h^{22}\,854\,513}{1\,554\,432} \\ &\quad + \frac{h^{26}\,8\,553\,103}{319\,488} - \frac{h^{30}\,8\,615\,841\,276\,005}{3\,519\,774\,720} \\ &\quad + \cdots + (-1)^{\frac{s-1}{2}} h^{2s} b_{2s}(2s-1)!\,2^{2-s} + R(h,2s), \quad s = 1,3,5,\cdots. \end{aligned} \tag{2.4.6}$$

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$$r(h) < 4h^{-1/2} 10^{\left(1 - \frac{30}{11h}\right)}. \tag{2.4.4}$$

Then using (2.4.4) and (2.3.16) we compute the values in Table 2.4.1.

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Hence, employing the Euler-Maclaurin Summation formula, we have

$$\begin{aligned} \pi &= h \sum_{i=0}^{n}{}'' \frac{4}{1+(ih)^2} \\ &\quad - \sum_{a=1}^{(s+1)/2} (-1)^a h^{4a-2} b_{4a-2} (4a-3)!\,2^{3-2a} + R(h,2s) \\ &= h \sum_{i=0}^{n}{}'' \frac{4}{1+(ih)^2} + \frac{h^2}{6} - \frac{h^6}{504} + \frac{h^{10}}{1056} - \frac{h^{14}}{384} \\ &\quad + \frac{h^{18}\,43\,867}{1\,838\,592} - \frac{h^{22}\,854\,513}{1\,554\,432} \\ &\quad + \frac{h^{26}\,8\,553\,103}{319\,488} - \frac{h^{30}\,8\,615\,841\,276\,005}{3\,519\,774\,720} \\ &\quad + \cdots + (-1)^{\frac{s-1}{2}} h^{2s} b_{2s} (2s-1)!\,2^{2-s} + R(h,2s), \quad s = 1,3,5,\cdots. \end{aligned} \tag{2.4.6}$$

Computation to 14 decimals with $h = 1/5$ and $s = 15$ in (2.4.6) gives

$$\pi - R\left(\frac{1}{5}, 17\right) = \frac{1}{5}\left(2 + \frac{100}{26} + \frac{100}{29} + \frac{100}{34} + \frac{100}{39} + 1\right)$$

$$+ \frac{5^{-2}}{6} - \frac{5^{-6}}{504} + \frac{5^{-10}}{1056} - \frac{5^{-14}}{384} + \cdots \tag{2.4.7}$$

$$= 3.141\ 592\ 653\ 590\ \underline{0}7.$$

The actual error is 2.8×10^{-13} while the error from Table 2.4.1 is 2.1×10^{-12}.

Finally we note in Table 2.4.1 that 50 decimals of π are guaranteed by taking $h = 1/19$ and $s = 59$ in (2.4.6). This requires 80 function evaluations (*fe*). It can be shown from (2.3.7) that 50 decimals of π are also guaranteed by taking $h = 1/29$ and $s = 25$. The computational cost is 55 *fe*.

Table 2.4.1 Computation of π

h	s	Upper bound for $r(h)$	*nfe*
1	3	7.50-2*	6
1/2	6	9.93-5	9
1/4	12	9.86-10	17
1/5	15	2.07-12	22
1/8	25	1.72-20	35
1/10	31	6.75-26	43
⋮	⋮	⋮	⋮
1/19	59	2.65-50	80

*This means 7.50×10^{-2}.

3. APPLICATIONS OF THE EULER-MACLAURIN SUMMATION FORMULA

3.1 QUADRATURE FORMULAS WITH ASYMPTOTIC EXPANSIONS

Sheppard [45], Becker [6], and Frame [18] suggested a class of quadrature formulas which are obtained by taking a weighted average of $T(h)$, $T(2h)$, $T(3h)$, $\cdots$ with weights selected to eliminate one or more of the terms containing $D_1, D_3, D_5, \cdots$. This is accomplished as follows.

Let $a_1, a_2, \cdots, a_{s+1}$ be factors of $n = (b-a)/h$. As before we write $E_{2\beta-1} = h^{2\beta}D_{2\beta-1}$ and $\Delta_{2\beta-1} = b_{2\beta}E_{2\beta-1}$. Denote by $A^{a_1 a_2 \cdots a_{s+1}}_{2\beta_1-1, 2\beta_2-1, \cdots, 2\beta_{s-1}}(h)$ the approximation to the integral $I(f) = \int_a^b f(x)dx$ based on the weighted average of $T(a_1h), T(a_2h), \cdots, T(a_{s+1}h)$ which eliminates the terms $\Delta_{2\beta_j-1}$, $j = 1(1)s$, but possibly contains some derivative correction terms involving $\Delta_{2\gamma_1-1}, \cdots, \Delta_{2\gamma_t-1}$.

Without loss of generality, suppose that

$$\begin{aligned} 1 &\leqslant a_1 < a_2 < \cdots < a_{s+1} \leqslant n \\ 1 &\leqslant \beta_1 < \beta_2 < \cdots < \beta_s \\ 1 &\leqslant \gamma_1 < \gamma_2 < \cdots < \gamma_t . \end{aligned} \tag{3.1.1}$$

We wish to find constants w_i, $i = 1(1)s+1$ such that

$$\begin{aligned} A^{a_1 \cdots a_{s+1}}_{2\beta_1-1, \cdots, 2\beta_s-1}(h) &= \sum_{i=1}^{s+1} w_i T(a_i h) + \sum_{j=1}^{t} c_j \Delta_{2\gamma_j-1} \\ &= I(f) + c_0 \Delta_{2\gamma-1} + \cdots \end{aligned} \tag{3.1.2}$$

where γ is the smallest positive integer distinct from the β_i and γ_j, and c_j are certain constants. The constants w_i which are found by solving the linear system

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ a_1^{2\beta_1} & a_2^{2\beta_1} & \cdots & a_{s+1}^{2\beta_1} \\ \vdots & \vdots & & \vdots \\ a_1^{2\beta_s} & a_2^{2\beta_s} & \cdots & a_{s+1}^{2\beta_s} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_{s+1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{3.1.3}$$

determine the asymptotic expansion for the resulting quadrature formula:

$$A_{2\beta_1-1,\cdots,2\beta_s-1}^{a_1\cdots a_{s+1}}(h) = \sum_{i=1}^{s+1} w_i T(a_i h)$$

$$-\sum_{j=1}^{t}\left[\Delta_{2\gamma_j-1}\sum_{i=1}^{s+1} w_i a_i^{2\gamma_j}\right] \tag{3.1.4}$$

$$= I(f) + \sum_{\substack{k=\gamma \\ k\neq\beta_i \\ k\neq\gamma_j}}^{\infty}\left[\Delta_{2k-1}\sum_{i=1}^{s+1} w_i a_i^{2k}\right]$$

The principal error term is defined to be

$$\Delta_{2\gamma-1}\sum_{i=1}^{s+1} w_i a_i^{2\gamma}. \tag{3.1.5}$$

A quadrature formula of degree at least $2s+1$ may be constructed by taking $a_j = j$ and $\beta_k = k$ in (3.1.3). In this case, it is easily seen that the following matrix has rank $s+1$ and hence a unique solution exists.

$$\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 2^2 & 3^2 & \cdots & (s+1)^2 \\ 1 & 2^4 & 3^4 & \cdots & (s+1)^4 \\ \vdots & \vdots & \vdots & & \\ 1 & 2^{2s} & 3^{2s} & \cdots & (s+1)^{2s} \end{bmatrix} = [j^{2(i-1)}]_{ij} \tag{3.1.6}$$

The Vandermonde determinant associated with this matrix is nonzero:

$$\frac{1}{(s+1)!}\prod_{k=0}^{s}(2k+1)! \neq 0.$$

Thus there are countably many quadrature formulas in this class. Becker [6] conjectured but did not prove this result.

The principal error term is

$$\Delta_{2s-1} \sum_{i=1}^{s+1} w_i i^{2s} \tag{3.1.7}$$

and the asymptotic expansion is

$$\begin{aligned} A_{1,2,\cdots,s}^{1,2,\cdots,s+1}(h) &= \sum_{i=1}^{s+1} w_i(ih) \\ &= I(f) + \sum_{k=s}^{\infty} \left[\Delta_{2k-1} \sum_{i=1}^{s+1} w_i i^{2s} \right]. \end{aligned} \tag{3.1.8}$$

We hasten to point out that this may not be the best quadrature formula. A more efficient quadrature rule may be obtained by selecting $n = (b - a)/h$ to have as many factors as possible, $1 = a_1 < a_2 < \cdots < a_{s+1} = n$. This may be seen by comparing the principal error terms in the 7-point formulas A_{12}^{123} and A_{123}^{1236}, which are $h^6 D_5/840$ and $3h^8 D_7/2800$, respectively.

For reference we list in Tables 3.1.1 to 3.1.4 several formulas constructed by this method. The entries in the tables may be understood by comparing them with the derivative corrected (DC) Simpson's Rule where $h = (b - a)/2n$ and $f_i = a + ih$.

$$\begin{aligned} A_3^{12} &= [16T(h) - T(2h) - E_1]/15 \\ &= \frac{h}{15}[7f_0 + 16f_1 + 14f_2 + \cdots + 7f_{2n}] - \frac{1}{15}h^2[f'(b) - f'(a)] \\ &= I(f) - \frac{h^6 D_5}{9450} + \frac{h^8 D_7}{75\,600} - \frac{h^{10} D_9}{712\,800} + \cdots \\ &= \int_a^b f(x)dx + \sum_{s=3}^{\infty} h^{2s} b_{2s} D_{2s-1}(16 - 4^s)/15. \end{aligned} \tag{3.1.9}$$

The principal error is the first term in the asymptotic expansion, $-h^6 D_5/9450$.

Table 3.1.1 Derivation of Closed Quadrature Formulas*

Name	Rule	Abbrev	Factor of T_α	T_1	T_2	T_3	T_4	T_6	T_8	E_1
Trapezoidal	A^1	$T(h)$	1	1						
DC Trapezoidal	A^1	$T'(h)$	1	1						$\frac{-1}{12}$
Simpson	A_1^{12}	$S(h)$	$\frac{1}{3}$	4	-1					
DC Simpson	A_3^{12}	$S'(h)$	$\frac{1}{15}$	16	-1					$\frac{-1}{15}$
Simpson's Second	A_1^{13}	$U(h)$	$\frac{1}{8}$	9		-1				
DC Simpson's Second	A_3^{13}	$U'(h)$	$\frac{1}{80}$	81		-1				$\frac{-3}{40}$
5-Point	A_1^{14}		$\frac{1}{15}$	16			-1			
DC 5-Point	A_3^{14}		$\frac{1}{255}$	256			-1			$\frac{-4}{51}$
Boole	A_{13}^{124}	$B(h)$	$\frac{1}{45}$	64	-20		1			
DC Boole	A_{35}^{124}	$B'(h)$	$\frac{1}{945}$	1 024	-80		1			$\frac{-4}{63}$
Weddle	A_{13}^{123}	$V(h)$	$\frac{1}{10}$	15	-6	1				
DC Weddle	A_{35}^{123}	$V'(h)$	$\frac{1}{245}$	270	-27	2				$\frac{-3}{49}$
Newton-Cotes' 7-Pt.	A_{135}^{1236}	$N(h)$	$\frac{1}{840}$	1 296	-567	112		-1		
DC Newton-Cotes' 7-Pt.	A_{357}^{1236}	$N'(h)$	$\frac{1}{42\,000}$	46 656	-5 103	448		-1		$\frac{-3}{50}$
Romberg 9-Pt.	A_{135}^{1248}	$W(h)$	$\frac{1}{2\,835}$	4 096	-1 344		84		-1	
DC Romberg 9-Pt.	A_{357}^{1248}	$W'(h)$	$\frac{1}{240\,975}$	262 144	-21 504		336		-1	$\frac{-112}{1785}$

*DC denotes Derivative Corrected and $T_\alpha = T(\alpha h)$ and $E_1 = h^2 D_1$.

Table 3.1.2 Quadrature Weights and Derivative Correction Terms

Name	Rule	Abbrev	Factor of f_i	f_0	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	$f_{\alpha n}$	α	E_1
Trapezoidal	A^{1}	$T(h)$	h	$\frac{1}{2}$	1								$\frac{1}{2}$	1	
DC Trapezoidal	A^{1}	$T'(h)$	h	$\frac{1}{2}$	1								$\frac{1}{2}$	1	$\frac{-1}{12}$
Simpson	A_1^{12}	$S(h)$	$\frac{h}{3}$	1	4	2							1	2	
DC Simpson	A_3^{12}	$S'(h)$	$\frac{h}{15}$	7	16	14							7	2	$\frac{-1}{15}$
Simpson's Second	A_1^{13}	$U(h)$	$\frac{3h}{8}$	1	3	3	2						1	3	
DC Simpson's Second	A_3^{13}	$U'(h)$	$\frac{3h}{80}$	13	27	27	26						13	3	$\frac{-3}{40}$
5–Point	A_1^{14}		$\frac{2h}{15}$	3	8	8	8	6					3	4	
DC 5–Point	A_3^{14}		$\frac{2h}{255}$	63	128	128	128	126					63	4	$\frac{-4}{51}$
Boole	A_{13}^{124}	$B(h)$	$\frac{2h}{45}$	7	32	12	32	14					7	4	
DC Boole	A_{35}^{124}	$B'(h)$	$\frac{2h}{945}$	217	512	432	512	434					217	4	$\frac{-4}{63}$
Weddle	A_{13}^{123}	$V(h)$	$\frac{3h}{10}$	1	5	1	6	1	5	2			1	6	
DC Weddle	A_{35}^{123}	$V'(h)$	$\frac{3h}{245}$	37	90	72	92	72	90	74			37	6	$\frac{-3}{49}$
Newton-Cotes' 7-Pt.	A_{135}^{1236}	$N(h)$	$\frac{h}{140}$	41	216	27	272	27	216	82			41	6	
DC Newton-Cotes' 7-Pt.	A_{357}^{1236}	$N'(h)$	$\frac{h}{7000}$	3 149	7 776	6 075	8 000	6 075	7 776	6 298			3 149	6	$\frac{-3}{50}$
Romberg 9-Pt.	A_{135}^{1248}	$W(h)$	$\frac{4h}{2835}$	217	1 024	352	1 024	436	1 024	352	1 024	434	217	8	
DC Romberg 9-Pt.	A_{357}^{1248}	$W'(h)$	$\frac{h}{240\,975}$	27 559	65 536	54 784	65 536	55 120	65 536	54 784	65 536	55 118	27 559	8	$\frac{-112}{1785}$

$f_i = a + ih$, and $h = (b - a)/\alpha n$.

Table 3.1.3 Prinicipal Errors and General Terms in the Asymptotic Expansions*

Name	Rule	Abbrev	Principal Error	General Term in Asymptotic Expansion
Trapezoidal	A^1	$T(h)$	$E_1/12$	Δ_{2S-1}
DC Trapezoidal	A^1	$T'(h)$	$-E_3/720$	Δ_{2S-1}
Simpson	A_1^{12}	$S(h)$	$E_3/180$	$\Delta_{2S-1}\ [4-4^S]/3$
DC Simpson	A_3^{12}	$S'(h)$	$-E_5/9\,450$	$\Delta_{2S-1}\ [16-4^S]/15$
Simpson's Second	A_1^{13}	$U(h)$	$E_3/80$	$\Delta_{2S-1}\ [9-9^S]/8$
DC Simpson' Second	A_3^{13}	$U'(h)$	$-3E_5/1\,120$	$\Delta_{2S-1}\ [81-9^S]/80$
5-Point	A_1^{14}		$E_3/45$	$\Delta_{2S-1}\ [16-16^S]/15$
DC 5-Point	A_3^{14}		$-8E_5/16\,065$	$\Delta_{2S-1}\ [256-16^S]/255$
Boole	A_{13}^{124}	$B(h)$	$2E_5/945$	$\Delta_{2S-1}\ [64-20(4^S)+16^S]/45$
DC Boole	A_{35}^{124}	$B'(h)$	$-4E_7/99\,225$	$\Delta_{2S-1}\ [1024-80(4^S)+16^S]/945$
Weddle	A_{13}^{123}	$V(h)$	$E_5/840$	$\Delta_{2S-1}\ [15-6(4^S)+9^S]/10$
DC Weddle	A_{35}^{123}	$V'(h)$	$-3E_7/137\,200$	$\Delta_{2S-1}\ [270-27(4^S)+2(9^S)]/245$
Newton-Cotes' 7-Pt.	A_{135}^{1236}	$N(h)$	$3E_7/2\,800$	$\Delta_{2S-1}\ [1296-567(4^S)+112\,(9^S)-36^S]/840$
DC Newton-Cotes' 7-Pt.	A_{357}^{1236}	$N'(h)$	$-3E_9/154\,000$	$\Delta_{2S-1}\ [46\,656-5\,103(4^S)+448(9^S)-36^S]/42\,000$
Romberg 9-Pt.	A_{135}^{1248}	$W(h)$	$16E_7/4\,725$	$\Delta_{2S-1}\ [4096-1344(4^S)+84(16^S)-64^S]/2\,835$
DC Romberg 9-Pt.	A_{357}^{1248}	$W'(h)$	$-512E_9/7\,952\,175$	$\Delta_{2S-1}\ [262\,144-21\,504(4^S)+336(16^S)-64^S]/240\,975$

*$E_{2S-1} = h^{2S}D_{2S-1}$ and $\Delta_{2S-1} = b_{2S}E_{2S-1}$.

Table 3.1.4 Leading Terms in the Asymptotic Expansions*

Name	Rule	Abbrev	E_1	E_3	E_5	E_7	E_9
Trapezoidal	A^{1}	$T(h)$	$\frac{1}{12}$	$\frac{-1}{720}$	$\frac{1}{30\,240}$	$\frac{-1}{1\,209\,600}$	$\frac{1}{47\,900\,160}$
DC Trapezoidal	A^{1}	$T'(h)$		$\frac{-1}{720}$	$\frac{1}{30\,240}$	$\frac{-1}{1\,209\,600}$	$\frac{1}{47\,900\,160}$
Simpson	A_1^{12}	$S(h)$		$\frac{1}{180}$	$\frac{-1}{1\,512}$	$\frac{1}{14\,400}$	$\frac{-17}{2\,395\,008}$
DC Simpson	A_3^{12}	$S'(h)$			$\frac{-1}{9\,450}$	$\frac{1}{75\,600}$	$\frac{-1}{712\,800}$
Simpson's Second	A_1^{13}	$U(h)$		$\frac{1}{80}$	$\frac{-1}{336}$	$\frac{13}{19\,200}$	$\frac{-41}{266\,112}$
DC Simpson's Second	A_3^{13}	$U'(h)$			$\frac{-3}{11\,200}$	$\frac{3}{44\,800}$	$\frac{-13}{844\,800}$
5-Point	A_1^{14}			$\frac{1}{45}$	$\frac{-17}{1\,890}$	$\frac{13}{3\,600}$	$\frac{-4369}{2\,993\,760}$
DC 5-Point	A_3^{14}				$\frac{-8}{16\,065}$	$\frac{17}{80\,325}$	$\frac{-13}{151\,470}$
Boole	A_{13}^{124}	$B(h)$			$\frac{2}{945}$	$\frac{-1}{900}$	$\frac{119}{249\,480}$
DC Boole	A_{35}^{124}	$B'(h)$				$\frac{-4}{99\,225}$	$\frac{2}{93\,555}$
Weddle	A_{13}^{123}	$V(h)$			$\frac{1}{840}$	$\frac{-1}{2\,400}$	$\frac{7}{63\,360}$
DC Weddle	A_{35}^{123}	$V'(h)$				$\frac{-3}{137\,200}$	$\frac{1}{129\,360}$
Newton-Cotes' 7-Pt.	A_{135}^{1236}	$N(h)$				$\frac{3}{2\,800}$	$\frac{-5}{3\,696}$
DC Newton-Cotes' 7-Pt.	A_{357}^{1236}	$N'(h)$					$\frac{-3}{154\,000}$
Romberg 9-Pt.	A_{135}^{1248}	$W(h)$				$\frac{16}{4\,725}$	$\frac{-136}{18\,711}$
DC Romberg 9-Pt.	A_{357}^{1248}	$W'(h)$					$\frac{-512}{7\,952\,175}$

*$E_{2S-1} = h^{2S} D_{2S-1}$.

Uspensky [52] uses the expansion of a function in terms of Bernoulli polynomials (see Krylov [27]) to derive asymptotic expansions for the trapezoidal, Simpson's, Simpson's Second, Boole's, and Newton-Cotes' 7-Point rules. Except for these Newton-Cotes' rules, Weddle's rule, the DC trapezoidal rule, and the DC Simpson's rule given by Tanimoto [50], the asymptotic expansions of this section are believed to be new; the derivation is based on the Euler-Maclaurin Summation formula.

Becker [6] constructed Simpson's, Boole's, Newton-Cotes' 7-Point, Weddle's, Romberg's 9-Point, and several other rules, but did not construct the corresponding derivative corrected rules as we have done.

3.2 ERROR ESTIMATES

The quadrature error in (3.1.4) may be estimated from the principal error term by

$$|I(f) - A_{\beta_1 \cdots \beta_s}^{a_1 \cdots a_{s+1}}(h)| \approx (b-a)|b_{2\gamma}|h^{2\gamma}M_{2\gamma}\sum_{i=1}^{s+1} |w_i|a_i^{2\gamma}. \tag{3.2.1}$$

Here we have replaced $D_{2\gamma-1}$ in (3.1.5) with $(b-a)M_{2\gamma}$. Also, as before,

$$\gamma = \min[I^+ - \{\beta_1, \cdots, \beta_s, \gamma_1, \cdots, \gamma_t\}]. \tag{3.2.2}$$

For example, let us compare Simpson's formula $S(h)$ with the DC Simpson's formula $S'(h)$. The error in Simpson's formula is less than $(b-a)h^4M_4/180$, whereas, the error in the DC Simpson's formula is less than $(b-a)h^6M_6/9450$. Now if

$$\frac{2h^2M_6}{105\,M_4} < 1 \tag{3.2.3}$$

then this additional accuracy of fifth-order vs. third-order is gained at the one-time minimal cost of computing the correction term $-h^2[f'(b) - f'(a)]/15$.

3.3 NEWTON-COTES FORMULAS

Examination of Tables 3.1.1 to 3.1.4 reveals that we have obtained asymptotic expansions for five of the Newton-Cotes' quadrature formulas: the trapezoidal rule, $T(h)$, Simpson's rule, $S(h)$, Simpson's Second rule, $U(h)$, Boole's rule, $B(h)$, and the Newton-Cotes' 7-Point rule, $N(h)$.

Examination of

$$\begin{aligned} A_1^{15}(h) &= [26\,T(h) - T(5h)]/25 \\ &= \frac{h}{50}[21f_0 + 52f_1 + 52f_2 + 52f_3 + 52f_4 + 42f_5 + \cdots + 21f_n] \qquad (3.3.1) \\ &= I(f) + 599h^4D_3/18\,000 - \cdots \end{aligned}$$

reveals that it is impossible using the technique described in Section 3.1 to obtain the 6-point Newton-Cotes' rule. Therefore, this class of quadrature formulas is not merely a restatement of the Newton-Cotes' rules.

As previously noted, Uspensky [52] shows how another technique may be used to obtain an asymptotic expansion for any Newton-Cotes' quadrature formula.

3.4 THE MIDPOINT RULE AND SOME OPEN FORMULAS

An asymptotic expansion for the midpoint or centroid formula, $C(h)$, may be derived from the Euler-Maclaurin Summation formula by writing

$$\begin{aligned} C(h) &= 2T(h/2) - T(h) \\ &= h\sum_{i=0}^{n} f(a+ih/2) \\ &= \int_a^b f(x)dx - E_1/24 + 7E_3/5760 \qquad (3.4.1) \\ &\quad -31E_5/967\,680 + \cdots + (2^{1-2s}-1)E_{2s-1}b_{2s} \\ &\quad + R(h,2s) \end{aligned}$$

where $h = (b - a)/n$ and the absolute error $|R(h, 2s)| = |R(h, 2s+1)|$ is estimated by

$$|R(h,2s+1)| = \left| \int_0^1 [2F_{h/2}^{(2s+1)}(t) - F_h^{(2s+1)}]B_{2s+1}(t)dt \right|$$

$$\leqslant [1 + 2^{-(2s+1)}] \frac{\pi^4}{15\sqrt{6}} (b - a) M_{2s+2}^{\bullet} \left(\frac{h}{2\pi}\right)^{2s+2}. \tag{3.4.2}$$

Of course, (2.3.5) and (2.3.6) may also be employed to obtain additional estimates for $R(h, 2s)$. As before,

$$M_{2s} = \max_{a \leqslant x \leqslant b} |f^{(2s)}(x)| \tag{3.4.3}$$

and

$$D_{2s-1} = f^{(2s-1)}(b) - f^{(2s-1)}(a)$$

$$E_{2s-1} = h^{2s}D_{2s-1} \tag{3.4.4}$$

$$\Delta_{2s-1} = b_{2s}E_{2s-1}.$$

From (3.4.1) we immediately obtain the derivative corrected (DC) midpoint formula

$$C'(h) = h \sum_{i=0}^{n} f(a + ih/2) + E_1/24$$

$$= \int_a^b f(x)dx + 7E_3/5760 - 31E_5/967\,680 \tag{3.4.5}$$

$$+ \cdots + (2^{1-2s} - 1)h^{2s}b_{2s}D_{2s-1} + R(h,2s).$$

The error $R(h, 2s)$ may be estimated by

$$|R(h, 2s)| \leqslant 3(b - a)M_4(h/2\pi)^4. \tag{3.4.6}$$

Here 3 is an approximation for $(3\pi^4/40\sqrt{6})$.

The principal error term of the DC midpoint quadrature formula is $7h^4D_3/5760$. This compares favorably with the Simpson's principal error term, $h^4D_3/180$.

Squire [47] observed that Simpson's rule is "probably the most widely used integration formula." Thus it is of interest to compare the third-order DC midpoint and Simpson's quadrature formulas.

Clearly the DC midpoint rule is easier to apply than Simpson's rule since the weights in the former are unity whereas there are three different weights for (composite) Simpson's formula.

If n represents the number of times the basic or holistic quadrature rule is applied, then traditionally, for Simpson's rule, $h = (b - a)/2n$ while for the midpoint rule, $h = (b - a)/n$. Thus one is tempted to compare the midpoint and Simpson results for the same step size h. Rather one should compare results when the holistic rule is applied an equivalent number of times, n. (Note that this is done in Chapters 6 and 7.) Milne [36] also discusses this.

When this method of comparison is used, then one sees that for n applications, the DC midpoint principal error is exactly 3.5 times the Simpson principal error. However, the DC midpoint rule uses only $n+2$ function evaluations (counting a derivative evaluation as one function evaluation), while Simpson's rule requires $2n + 1$ function evaluations.

Therefore, for the same order of magnitude error, the Derivative Corrected midpoint formula (3.4.4) requires approximately half the number of function evaluations as Simpson's rule. This represents a considerable savings in computer time.

Table 3.4.1 The Midpoint, DC Midpoint, and Simpson's Rules Applied to $\int_3^6 \frac{dx}{x} = \ln 2$

n	Midpoint		DC Midpoint		Simpson	
	Error	*nfe*	Error	*nfe*	Error	*nfe*
3	3.39-3*	3	−7.97-5	5	−2.26-5	7
6	8.63-4	6	−5.20-6	8	−1.48-6	13
12	2.17-4	12	−3.28-7	14	−9.41-8	25
24	5.42-5	24	−2.08-8	26	−6.20-9	49

*This means 3.39×10^{-3}.

As can be seen in the Table 3.4.1, for $n = 6$ the DC midpoint rule produces an error of 5.20×10^{-6} using only 8 function evaluations while Simpson's rule requires 13 function evaluations to produce an error of 1.48×10^{-6}.

Thus, in situations where Simpson's rule is considered adequate for the approximation of a definite integral, the DC midpoint rule should be considered as a viable alternative to Simpson's rule.

Next we use the midpoint rule (3.4.1) to derive several open formulas based on the methods of Section 3.2. A numerical integration formula is defined to be open if all of the nodes are interior to the domain of integration.

Let $a_1, \cdots, a_{s+1}$ be factors of $n = (b-a)/h$. Denote by $Q^{a_1 \cdots a_{s+1}}_{2\beta_1-1,\cdots,2\beta_s-1}(h)$ the approximation to $I(f) = \int_a^b f(x)dx$ based on the weighted average $C(a_1h), \cdots, C(a_{s+1}h)$ which eliminates the terms containing $\Delta_{2\beta_1-1}, \cdots, \Delta_{2\beta_s-1}$, but possibly contains t derivative correction terms involving $\Delta_{2\gamma_1-1}, \cdots, \Delta_{2\gamma_t-1}$.

Assuming that (3.1.1) holds, we seek constants w_i, $i = 1(1)s+1$, such that

$$\begin{aligned} Q^{a_1 \cdots a_{s+1}}_{2\beta_1-1,\cdots,2\beta_s-1}(h) &= \sum_{i=1}^{s+1} w_i C(a_ih) + \sum_{j=1}^{t} c_j \Delta_{2\gamma_j-1} \\ &= I(f) + c_0(2^{1-2\gamma}-1)\Delta_{2\gamma-1} + \cdots . \end{aligned} \tag{3.4.7}$$

Here γ is the smallest positive integer distinct from the β_i and γ_j and c_j are certain constants. Now using (3.1.3) to find the numbers w_i, we obtain an asymptotic expansion for the resulting quadrature formula

$$\begin{aligned} Q^{a_1 \cdots a_{s+1}}_{2\beta_1-1,\cdots,2\beta_s-1}(h) &\doteq \sum_{i=1}^{s+1} w_i C(a_ih) - \sum_{j=1}^{t} \left[(2^{1-2\gamma_j}-1)\Delta_{2\gamma_j-1} \sum_{i=1}^{s+1} w_i a_i^{2\gamma_j} \right] \\ &= \int_a^b f(x)dx + \sum_{\substack{k=\gamma \\ k\neq\beta_i \\ k\neq\gamma_j}}^{\infty} \left[(2^{1-2k}-1)\Delta_{2k-1} \sum_{i=1}^{s+1} w_i a_i^{2k} \right] \end{aligned} \tag{3.4.8}$$

having the principal error

$$(2^{1-2\gamma} - 1)\Delta_{2\gamma-1} \sum_{i=1}^{s+1} w_i a_i^{2\gamma} \tag{3.4.9}$$

Several open and derivative corrected open quadrature rules obtained by this technique are presented in Tables 3.4.2 to 3.4.5.

For reference we state the open quadrature formula Q_3^{12} which is the analog of the derivative corrected Simpson's formula.

$$\begin{aligned}
Q_3^{12} &= S_0'(h) \\
&= [16C(h) - C(2h) - E_1/2]/15 \\
&= \frac{2h}{15}[2f(a+h/2) - f(a+h) + 2f(a+3h/2) + \cdots \\
&\quad + 2f(b-3h/2) - f(b-h) + 2f(b-h/2)] + \frac{h^2}{30}[f'(b) - f'(a)] \qquad (3.4.10) \\
&= I(f) + \frac{31h^6 D_5}{302\,400} - \frac{127\,h^8 D_7}{9\,676\,800} + \cdots \\
&= \int_a^b f(x)dx + \sum_{s=3}^{\infty} h^{2s} b_{2s} D_{2s-1} (2^{1-2s} - 1)(16 - 4^s)/15.
\end{aligned}$$

The open quadrature formula $Q_{2\beta_1-1,\cdots,2\beta_s-1}^{a_1,\cdots,a_{s+1}}(h)$ based on the asymptotic expansion of the midpoint rule is the analog of the closed formula $A_{2\beta_1-1,\cdots,2\beta_s-1}^{a_1,\cdots,a_{s+1}}(h)$ which is based on the Euler-Maclaurin Summation formula.

In particular, the open formulas S_0, U_0, B_0, V_0, N_0, and W_0 are the analogs of Simpson's, Simpson's Second, Boole's, Weddle's, Newton-Cotes' 7-point, and Romberg's 9-point formulas, respectively.

Finally we note the following relationships:

$$\begin{aligned}
S_0(h) &= [4C(h) - C(2h)]/3 \\
B_0(h) &= [16S_0(h) - S_0(2h)]/15 \qquad (3.4.11) \\
W_0(h) &= [64B_0(h) - B_0(2h)]/63.
\end{aligned}$$

Table 3.4.2 Derivation of Open Quadrature Formulas*

Rule	Abbrev	Factor of C_a	C_1	C_2	C_3	C_4	C_6	C_8	E_1
Q^1	$C(h)$	1	1						
Q^1	$C'(h)$	1	1						$\frac{1}{24}$
Q_1^{12}	$S_o(h)$	$\frac{1}{3}$	4	-1					
Q_3^{12}	$S'_o(h)$	$\frac{1}{15}$	16	-1					$\frac{1}{30}$
Q_1^{13}	$U_o(h)$	$\frac{1}{8}$	9		-1				
Q_3^{13}	$U'_o(h)$	$\frac{1}{80}$	81		-1				$\frac{3}{80}$
Q_{13}^{124}	$B_o(h)$	$\frac{1}{45}$	64	-20		1			
Q_{35}^{124}	$B'_o(h)$	$\frac{1}{945}$	1 024	-80		1			$\frac{2}{63}$
Q_{13}^{123}	$V_o(h)$	$\frac{1}{10}$	15	-6	1				
Q_{35}^{123}	$V'_o(h)$	$\frac{1}{245}$	270	-27	2				$\frac{3}{98}$
Q_{135}^{1236}	$N_o(h)$	$\frac{1}{840}$	1 296	-567	112		-1		
Q_{357}^{1236}	$N'_o(h)$	$\frac{1}{42\,000}$	46 656	-5 103	448		-1		$\frac{3}{100}$
Q_{135}^{1248}	$W_o(h)$	$\frac{1}{2\,835}$	4 096	-1 344		84		-1	
Q_{357}^{1248}	$W'_o(h)$	$\frac{1}{240\,975}$	262 144	-21 504		336		-1	$\frac{56}{1\,785}$

*$C_a = C(ah)$ and $E_1 = h^2 D_1$.

Table 3.4.3 Quadrature Weights and Derivative Correction Terms

Rule	Abbrev	Factor of f_i	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9	f_{10}	f_{11}	f_{12}	f_{13}	f_{14}	f_{15}	E_1
Q^1	$C(h)$	h	1															
Q^1	$C'(h)$	h	1															$\frac{1}{24}$
Q_1^{12}	$S_o(h)$	$\frac{2h}{3}$	2	−1	2													
Q_3^{12}	$S_o'(h)$	$\frac{2h}{15}$	8	−1	8													$\frac{1}{30}$
Q_1^{13}	$U_o(h)$	$\frac{3h}{8}$	3		2		3											
Q_3^{13}	$U_o'(h)$	$\frac{3h}{80}$	27		26		27											$\frac{3}{80}$
Q_{13}^{124}	$B_o(h)$	$\frac{4h}{45}$	16	−10	16	1	16	−10	16									
Q_{35}^{124}	$B_o'(h)$	$\frac{4h}{945}$	256	−40	256	1	256	−40	256									$\frac{2}{63}$
Q_{13}^{123}	$V_o(h)$	$\frac{3h}{10}$	5	−4	6		5	−4	5		6	−4	5					
Q_{35}^{123}	$V_o'(h)$	$\frac{3h}{245}$	135	−18	91		135	−18	135		91	−18	135					$\frac{3}{98}$
Q_{135}^{1236}	$N_o(h)$	$\frac{h}{140}$	216	−189	272		216	−190	216		272	−189	216					
Q_{357}^{1236}	$N_o'(h)$	$\frac{h}{7000}$	7 776	−1 701	8 000		7 776	−1 702	7 776		8 000	−1 701	7 776					$\frac{3}{100}$
Q_{135}^{1248}	$W_o(h)$	$\frac{8h}{2835}$	512	−336	512	42	512	−336	512	−1	512	−336	512	42	512	−336	512	
Q_{357}^{1248}	$W_o'(h)$	$\frac{8h}{240975}$	32 768	−5 376	32 768	168	32 768	−5 376	32 768	−1	32 768	−5 376	32 768	168	32 768	−5 376	32 768	$\frac{56}{1785}$

$f_i = a + ih/2$ where $h = (b - a)/\alpha n$.

Table 3.4.4 Prinicpal Errors and General Terms in the Asymptotic Expansions*

Rule	Abbrev	Principal Error	General Term in Asymptotic Expansion
Q^1	$C(h)$	$-E_1/24$	$\Delta_{2S-1}(2^{1-2S}-1)$
Q^1	$C'(h)$	$7E_3/5\,760$	$\Delta_{2S-1}(2^{1-2S}-1)$
Q_1^{12}	$S_o(h)$	$-7E_3/1\,440$	$\Delta_{2S-1}(2^{1-2S}-1)[4-4^S]/3$
Q_3^{12}	$S_o'(h)$	$31E_5/302\,400$	$\Delta_{2S-1}(2^{1-2S}-1)[16-4^S]/15$
Q_1^{13}	$U_o(h)$	$-7E_3/640$	$\Delta_{2S-1}(2^{1-2S}-1)[9-9^S]/8$
Q_3^{13}	$U_o'(h)$	$93E_5/35\,840$	$\Delta_{2S-1}(2^{1-2S}-1)[81-9^S]/80$
Q_{13}^{124}	$B_o(h)$	$-31E_5/15\,120$	$\Delta_{2S-1}(2^{1-2S}-1)[64-20(4^S)+16^S]/45$
Q_{35}^{124}	$B_o'(h)$	$127E_7/3\,175\,200$	$\Delta_{2S-1}(2^{1-2S}-1)[1\,024-80(4^S)+16^S]/945$
Q_{13}^{123}	$V_o(h)$	$-31E_5/26\,880$	$\Delta_{2S-1}(2^{1-2S}-1)[15-6(4^S)+9^S]/10$
Q_{35}^{123}	$V_o'(h)$	$381E_7/17\,561\,600$	$\Delta_{2S-1}(2^{1-2S}-1)[270-27(4^S)+2(9^S)]/245$
Q_{135}^{1236}	$N_o(h)$	$-381E_7/358\,400$	$\Delta_{2S-1}(2^{1-2S}-1)[1\,296-567(4^S)+112(9^S)-36^S]/840$
Q_{357}^{1236}	$N_o'(h)$	$1533E_9/78\,848\,000$	$\Delta_{2S-1}(2^{1-2S}-1)[46\,656-5\,103(4^S)+488(9^S)-36^S]/42\,000$
Q_{135}^{1248}	$W_o(h)$	$-127E_7/37\,800$	$\Delta_{2S-1}(2^{1-2S}-1)[4\,096-1\,344(4^S)+84(16^S)-64^S]/2\,835$
Q_{357}^{1248}	$W_o'(h)$	$511E_9/7\,952\,175$	$\Delta_{2S-1}(2^{1-2S}-1)[262\,144-21\,504(4^S)+336(16^S)-64^S]/240\,975$

*$E_{2S-1} = h^{2S} D_{2S-1}$ and $\Delta_{2S-1} = b_{2S} E_{2S-1}$.

Table 3.4.5 Leading Terms in the Asymptotic Expansions*

Rule	Abbrev	E_1	E_3	E_5	E_7	E_9
Q^1	$C(h)$	$\frac{-1}{24}$	$\frac{7}{5\,760}$	$\frac{-31}{967\,680}$	$\frac{127}{154\,828\,800}$	$\frac{-511}{24\,524\,881\,900}$
Q^1	$C'(h)$		$\frac{7}{5\,760}$	$\frac{-31}{967\,680}$	$\frac{127}{154\,828\,800}$	$\frac{-511}{24\,524\,881\,900}$
Q_1^{12}	$S_o(h)$		$\frac{-7}{1\,440}$	$\frac{31}{48\,384}$	$\frac{-127}{1\,843\,200}$	$\frac{1241}{175\,177\,728}$
Q_3^{12}	$S_o'(h)$			$\frac{31}{302\,400}$	$\frac{-127}{9\,676\,800}$	$\frac{511}{364\,953\,600}$
Q_1^{13}	$U_o(h)$		$\frac{-7}{640}$	$\frac{31}{10\,752}$	$\frac{-1651}{2\,457\,600}$	$\frac{2993}{19\,464\,192}$
Q_3^{13}	$U_o'(h)$			$\frac{93}{358\,400}$	$\frac{-381}{5\,734\,400}$	$\frac{6643}{432\,537\,600}$
Q_{13}^{124}	$B_o(h)$			$\frac{-31}{15\,120}$	$\frac{127}{115\,200}$	$\frac{-8687}{18\,247\,680}$
Q_{35}^{124}	$B_o'(h)$				$\frac{127}{3\,175\,200}$	$\frac{-73}{3\,421\,440}$
Q_{13}^{123}	$V_o(h)$			$\frac{-31}{26\,880}$	$\frac{127}{307\,200}$	$\frac{-3577}{32\,440\,320}$
Q_{35}^{123}	$V_o'(h)$				$\frac{381}{17\,561\,600}$	$\frac{-73}{9\,461\,760}$
Q_{135}^{1236}	$N_o(h)$				$\frac{-381}{358\,400}$	$\frac{365}{270\,336}$
Q_{357}^{1236}	$N_o'(h)$					$\frac{219}{11\,264\,000}$
Q_{135}^{1248}	$W_o(h)$				$\frac{-127}{37\,800}$	$\frac{1241}{171\,072}$
Q_{357}^{1248}	$W_o'(h)$					$\frac{73}{581\,644\,800}$

*$E_{2S-1} = h^{2S} D_{2S-1}$.

For the derivative corrected formulas we have

$$\begin{aligned} S_0'(h) &= [16C'(h) - C'(2h)]/15 \\ B_0'(h) &= [64S_0'(h) - S_0'(2h)]/63 \\ W_0'(h) &= [256B_0'(h) - B_0'(2h)]/255. \end{aligned} \tag{3.4.12}$$

This leads to the observation that the derivative corrected Romberg quadrature to be defined in Section 3.6 may be based on the asymptotic expansion for the midpoint rule, (3.4.1), in place of the Euler-Maclaurin Summation formula. In this case the first 4 columns of the "open Romberg" table are given by the open quadrature rules $C(h), S_0(h), B_0(h)$, and $W_0(h)$, respectively.

3.5 ROMBERG QUADRATURE

The Euler-Maclaurin Summation formula is a tool of strategic theoretical importance. Indeed, Romberg [44] proposed a new class of quadrature formulas for a finite closed interval $[a,b]$ based on Richardson's extrapolation technique [24, 43] applied to the Euler-Maclaurin formula. It involves repeated halvings of the integration interval and successive elimination of higher order terms in the Euler-Maclaurin expansion.

An extensive discussion of the theory is given by Bauer, Rutishauser, and Stiefel [5].

Romberg concluded that Richardson's deferred approach to the limit would improve the accuracy of the trapezoidal rule.

$$T(h) = h\left[\frac{1}{2}f_0 + f_1 + \cdots + \frac{1}{2}f_n\right] = h\sum_{i=0}^{n}{}'' f(a+ih). \tag{3.5.1}$$

For $n = (b-a)/h$ even, he obtained Simpson's formula by writing

$$S(h) = [4T(h) - T(2h)]/3. \tag{3.5.2}$$

Next for n a multiple of 4 he obtained the Newton-Cotes' formula of order 6, Boole's Rule:

$$B(h) = [16S(h) - S(2h)]/15. \tag{3.5.3}$$

In the next step Romberg obtained the formula

$$\begin{aligned} W(h) &= [64B(h) - B(2h)]/63 \\ &= \frac{4h}{2835}[217f_0 + 1024f_1 + 352f_2 + 1024f_3 \\ &\quad + 436f_4 + 1024f_5 + 352f_6 + 1024f_7 + 434f_8 + \cdots + 217f_n] \end{aligned} \tag{3.5.4}$$

which is not a Newton-Cotes' quadrature rule. Thus Romberg's method is not a reformulation of the Newton-Cotes' formulas. Apparently, $W(h)$ was first derived by Sheppard [45] and later rediscovered by Becker [6].

Now let

$$T_{0k} = h \sum_{i=0}^{2k}{}'' f(a+ih) \tag{3.5.5}$$

be trapezoidal sums where $h = (b-a)/2^k$. Recalling the Euler-Maclaurin formula

$$T(h) = I(f) + \sum_{a=1}^{s} c_a h^{2a} - R(h,2s) \tag{3.5.6}$$

where $c_a = b_{2a} D_{2a-1}$, it is easy to understand the definition

$$T_{mk} = [4^m T_{m-1,k+1} - T_{m-1,k}]/[4^m - 1]. \tag{3.5.7}$$

In fact

$$T_{mk} = A_{1,2,\cdots,m}^{2^0,2^1,\cdots,2^m}\left(\frac{b-a}{2^k}\right), \quad m > 0. \tag{3.5.8}$$

From this the Romberg T-table is constructed:

$$\begin{array}{llll} T_{00} & & & \\ T_{01} & T_{11} & & \\ T_{02} & T_{12} & T_{22} & \\ T_{03} & T_{13} & T_{23} & T_{33} \\ \vdots & \vdots & \vdots & \ddots \end{array} \tag{3.5.9}$$

We have already seen that the first three columns are the trapezoidal, Simpson, and Boole's values, respectively.

Bauer, Rutishauser, and Stiefel [5] show for any $f \in C^{2m+2}[a,b]$ there is a $\zeta \in [0,1]$ such that

$$|T_{mk} - I(f)| \leqslant \frac{(b-a)B_{2m+2}|f^{(2m+2)}(\zeta)|}{(2m+2)!\, 2^{(2k-m)(m+1)}}. \tag{3.5.10}$$

Combining this result with lemma 2.1.2 we obtain a new and much more convenient error estimate for any entry in the Romberg table.

Theorem 3.5.1

If $f \in C^{2m+2}[a,b]$ then the error for any entry in the Romberg T-table may be estimated by

$$|T_{mk} - I(f)| \leq \frac{(b-a)M_{2m+2}}{45\,\pi^{2(m-1)}2^{(m+1)(2+2k-m)}} \tag{3.5.11}$$

where

$$M_{2m+2} = \max_{a \leq x \leq b} |f^{(2m+2)}(x)|. \tag{3.5.12}$$

3.6 DERIVATIVE CORRECTED ROMBERG QUADRATURE

Lanczos [28] shows how the addition of only one derivative correction term can significantly improve the accuracy of a quadrature formula at the minimal expense of a small increase in computational effort. He also states the derivative corrected (DC) trapezoidal and Simpson's Rules.

We note that the DC trapezoidal rule generates the DC Simpson's rule.

$$S'(h) = [16\,T'(h) - T'(2h)]/15 \tag{3.6.1}$$

which in turn generates the DC Boole's rule

$$B'(h) = [64\,S'(h) - S'(2h)]/63. \tag{3.6.2}$$

Next, the DC Boole's rule generates the DC 9-point Romberg formula

$$W'(h) = [256B'(h) - B'(2h)]/255 \tag{3.6.3}$$

which is distinct from any DC Newton-Cotes' rule.

This suggests a new quadrature scheme, the derivative corrected Romberg quadrature. Let

$$h = (b-a)/2^k \tag{3.6.4}$$

and

$$\begin{aligned} C^s_{0k} &= h \sum_{i=0}^{2^k}{}'' f(a+ih) - \sum_{a=1}^{s} \Delta_{2a-1} \\ &= T_{0k} - \Phi(h,s) \end{aligned} \tag{3.6.5}$$

be DC trapezoidal sums. Define

$$C^s_{mk} = (4^{m+s}C^s_{m-1,k+1} - C^s_{m-1,k})/(4^{m+s} - 1) \tag{3.6.6}$$

and construct the DC Romberg C^s-table

$$\begin{matrix} C^s_{00} \\ C^s_{01} & C^s_{11} \\ C^s_{02} & C^s_{12} & C^s_{22} \\ C^s_{03} & C^s_{13} & C^s_{23} & C^s_{33} \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{matrix} \tag{3.6.7}$$

The first column is the Euler-Maclaurin formula with $h = (b - a)/2^k$ and the m-th column, $m > 0$, is given by the quadrature formula

$$C^s_{mk} = A^{2^0,2^1,\cdots,2^m}_{s+1,s+2,\cdots,s+m}\left(\frac{b-a}{2^k}\right). \tag{3.6.8}$$

For the case $s = 1$, the first three columns of the C^1-table are the DC trapezoidal, DC Simpson's, and DC Boole's rules, respectively.

In general, comparing (3.5.8) with (3.6.8), we see that the m-th column of the C^s-table is the derivative corrected quadrature rule corresponding to the m-th column of the Romberg T-table.

3.7 A NUMERICAL EXAMPLE

To illustrate, we employ the Romberg and derivative corrected Romberg quadrature formulas to estimate the integral

$$\int_0^1 \frac{1}{2}\sin(\pi x)\pi dx = 1. \tag{3.7.1}$$

We note that

$$\begin{aligned} h &= 2^{-k} \\ D_{2a-1} &= (-1)^a \pi^{2a} \\ C^s_{0k} &= \pi 2^{1-k}\sum_{j=1}^{2^k-1}\sin(j\pi 2^{-k}) \\ \Phi(h,s) &= \sum_{a=1}^{s}(-1)^a\pi^{2a}2^{-2ka}b_{2a}. \end{aligned} \tag{3.7.2}$$

Table 3.7.1 Romberg Quadrature T-table for $\int_0^1 \frac{1}{2} \sin(\pi x) \pi dx = 1$

k \ m	0 (Trapezoidal)	1 (Simpson)	2 (Boole)	3 (Newton-Cotes' 7-Point)
0	0.000 000 000 000			
1	0.785 398 163 397	1.047 197 551 20		
2	0.948 059 448 969	1.002 279 877 49	0.999 285 365 912	
3	0.987 115 800 973	1.000 134 584 97	0.999 991 565 473	1.000 002 774 99

Table 3.7.2 Derivative Corrected Romberg Quadrature (s = 1) C^1-table

k \ m	0 (Corrected Trapezoidal)	1 (Corrected Simpson)	2 (Corrected Boole)	3 (Corrected Newton-Cotes' 7-Point)
0	0.822 467 033 424			
1	0.991 014 921 753	1.002 251 447 64		
2	0.999 463 638 558	1.000 026 886 34	0.999 991 575 848	
3	0.999 966 848 370	1.000 000 395 69	0.999 999 975 204	1.000 000 008 14

Table 3.7.3 Derivative Corrected Romberg Quadrature (s = 2) C^2-table

k \ m	0 (Corrected Trapezoidal)	1 (Corrected Simpson)	2 (Corrected Boole)	3 (Corrected Newton-Cotes' 7-Point)
0	0.957 757 437 638			
1	0.999 470 572 017	1.000 132 685 26		
2	0.999 992 116 699	1.000 000 395 19	0.999 999 876 401	
3	0.999 999 878 254	1.000 000 001 45	0.999 999 999 909	1.000 000 000 03

Table 3.7.4 Romberg Error for $\int_0^1 \frac{1}{2} \sin(\pi x)\pi dx = 1$

k \ m	0 (Trapezoidal)	1 (Simpson)	2 (Boole)	3 (Newton-Cotes' 7-Point)
0	1.00+0			
1	2.15-1	-4.72-2		
2	5.19-2	-2.28-3	7.15-4	
3	1.29-2	-1.35-4	8.44-6	-2.78-6

Table 3.7.5 Derivative Corrected Romberg Error ($s = 1$)

k \ m	0 (Corrected Trapezoidal)	1 (Corrected Simpson)	2 (Corrected Boole)	3 (Corrected Newton-Cotes' 7-Point)
0	1.78-1			
1	8.99-3	-2.25-3		
2	5.36-4	-2.69-5	8.42-6	
3	3.32-5	-3.96-7	2.48-8	-8.14-9

Table 3.7.6 Derivative Corrected Romberg Error ($s = 2$)

k \ m	0 (Corrected Trapezoidal)	1 (Corrected Simpson)	2 (Corrected Boole)	3 (Corrected Newton-Cotes' 7-Point)
0	4.22-2			
1	5.29-4	-1.33-4		
2	7.88-6	-3.95-7	1.24-7	
3	1.22-7	-1.45-9	9.09-11	-2.98-11

*This means 4.22×10^{-2}.

The values in the C^1-Table 3.7.2 show a marked improvement over those in the Romberg T-Table 3.7.1. For the calculation of the C^1-table, it should be emphasized that

$$D_1' = f'(1) - f'(0) \tag{3.7.3}$$

is computed only once, in fact before the calculation of the C^1-table commences. Thus the first derivative of the integrand is evaluated only at the two end points of the interval of integration.

The advantage of the derivative corrected Romberg quadrature over the classical Romberg quadrature is its increased accuracy and efficiency. Indeed, it can be shown that the m-th column of the C^s-table is given by a quadrature formula of order $h^{2(m+1)+2s}$ as compared with an $h^{2(m+1)}$ order for the m-th column of the Romberg T-table $(m=0,1,2,\cdots)$.

This improved accuracy is gained by the minimal cost of evaluating the derivative correction terms, D_{2a-1}', once. Moreover, the derivative corrected Romberg quadrature is appealing because the trapezoidal sums are closely related to Riemann sums, and the weights are easy to program. As noted on page 31, an extrapolation procedure may be applied to an asymptotic expansion for the midpoint rule in place of the trapezoidal rule.

4. FUNCTIONS OF TWO VARIABLES

4.1 THE EULER-MACLAURIN SUMMATION FORMULA

Let $C^{2s}[R]$ denote the set of functions $f(x,y)$ of two real variables where the partial derivatives (see 4.1.5) $f^{\alpha\beta}(x,y)$, $0 \leq \alpha, \beta \leq 2s$, exist and are continuous on the rectangle $R = [a,b] \times [c,d]$ and let $f(x,y) \in C^{2s}[R]$. We wish to estimate the integral

$$I(f) = \int_c^d \int_a^b f(x,y)dxdy. \tag{4.1.1}$$

Divide $[a,b]$ into n equal parts each of width $h = (b-a)/n$ by points $x_i = a + ih$ setting $x_0 = a$ and $x_n = b$. Similarly divide $[c,d]$ into m equal parts each of width $k = (d-c)/m$ by points $y_j = c + jk$ where $y_0 = c$ and $y_m = d$.

Now for $0 \leq t, u \leq 1$, average the values of $(b-a)(d-c)f$ in each subrectangle $R_{ij}, = [x_i, x_{i+1}] \times [y_j, y_{j+1}]$ at points at a distance of t from the left side and a distance of u from the bottom by writing

$$F_{hk}(t,u) = hk \sum_{j=0}^{m-1} \sum_{i=0}^{n-1} f(x_i + th, y_j + uk). \tag{4.1.2}$$

Then the double integral of this moving average over the unit square is exactly the integral $I(f)$ over the rectangle R:

$$\begin{aligned} &\int_0^1 \int_0^1 F_{hk}(t,u)dtdu \\ &= \sum_{j=0}^{m-1} \sum_{i=0}^{n-1} \int_0^1 \int_0^1 f(x_i + th, y_j + uk)hkdtdu \\ &= \sum_{j=0}^{m-1} \sum_{i=0}^{n-1} \int_{c+jk}^{c+(j+1)k} \int_{a+ih}^{a+(i+1)h} f(x,y)dxdy \\ &= \int_c^d \int_a^b f(x,y)dxdy. \end{aligned} \tag{4.1.3}$$

The average $T(h,k)$ is the (composite) trapezoidal rule:

$$T(h,k) = \frac{1}{4}[F(0,0) + F(1,0) + F(0,1) + F(1,1)]$$

$$= hk\sum_{j=0}^{m}{}''\sum_{i=0}^{n}{}'' f(x_i,y_j). \qquad (4.1.4)$$

The double primes on the summation signs indicate weights are to be assigned as indicated in Figure 4.1.1.

¼	½	. . .	½	¼
½	1	. . .	1	½
⋮	⋮		⋮	⋮
½	1	. . .	1	½
¼	½	. . .	½	¼

Figure 4.1.1 Trapezoidal Weights

The mid-value $F_{hk}(½, ½)$ is the composite centroid or midpoint rule and has been investigated by Good and Gaskins [20].

Before proceeding, we define some notation which will simplify the writing of the Euler-Maclaurin Summation formula. Let $\phi_\alpha(t)$ and $\psi_\alpha(u)$ represent the α-th Bernoulli polynomials in the variables t and u respectively, $\alpha \geqslant 1$.

For $1 \leqslant \alpha,\beta \leqslant 2s$ denote

$$f^{\alpha\beta}(x,y) = \mathcal{D}_2^{\beta}\mathcal{D}_1^{\alpha} f(x,y) \qquad (4.1.5)$$

and

$$d_{\alpha 0} = \sum_{j=0}^{m}{}''[f^{\alpha 0}(b,y_j) - f^{\alpha 0}(a,y_j)] \qquad (4.1.6)$$

$$d_{0\beta} = \sum_{i=0}^{n}{}''[f^{0\beta}(x_i,d) - f^{0\beta}(x_i,c)]$$

$$d_{\alpha\beta} = f^{\alpha\beta}(b,d) - f^{\alpha\beta}(b,c) - f^{\alpha\beta}(a,d) + f^{\alpha\beta}(a,c).$$

The double primes signify trapezoidal weights, that is, the first and last terms in each sum are to be assigned weights ½ and the remaining terms are assigned weights 1. The weight assignment is illustrated in Figure 4.1.2.

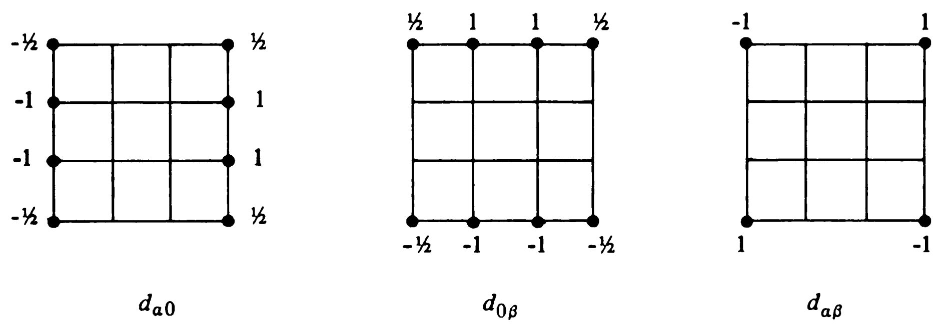


Figure 4.1.2 Partial Derivative Weight Assignments

Next for $\alpha, \beta = 1(2)2s - 1$ we define

$$D_{\alpha 0} = \frac{1}{2}[F^{\alpha 0}(1,1) + F^{\alpha 0}(1,0) - F^{\alpha 0}(0,1) - F^{\alpha 0}(0,0)]$$

$$D_{0\beta} = \frac{1}{2}[F^{0\beta}(1,1) - F^{0\beta}(1,0) + F^{0\beta}(0,1) - F^{0\beta}(0,0)] \tag{4.1.7}$$

$$D_{\alpha\beta} = F^{\alpha\beta}(1,1) - F^{\alpha\beta}(1,0) - F^{\alpha\beta}(0,1) + F^{\alpha\beta}(0,0)$$

and

$$I_{\alpha,0} = \frac{1}{2}\int_0^1 [F^{\alpha 0}(t,1) + F^{\alpha 0}(t,0)]\, \phi_\alpha(t)dt$$

$$I_{0,\beta} = \frac{1}{2}\int_0^1 [F^{0\beta}(1,u) + F^{0\beta}(0,u)]\, \psi_\beta(u)du$$

$$I_{2s,\beta} = \int_0^1 [F^{2s,\beta}(t,1) - F^{2s,\beta}(t,0)]\, \phi_{2s}(t)\mathrm{d}t \tag{4.1.8}$$

$$I_{\alpha,2s} = \int_0^1 [F^{\alpha,2s}(1,u) - F^{\alpha,2s}(0,u)]\, \psi_{2s}(u)du$$

$$I_{\alpha,\alpha} = \int_0^1\int_0^1 F^{\alpha\alpha}(t,u)\phi_\alpha(t)\psi_\alpha(u)dtdu.$$

Now since

$$F^{\alpha\beta}(t,u) = h^{\alpha+1}k^{\beta+1}\sum_{j=0}^{m-1}\sum_{i=0}^{n-1} f^{\alpha\beta}(x_i + th, y_j + uk) \tag{4.1.9}$$

we see that

$$\begin{aligned} D_{\alpha 0} &= h^{\alpha+1}kd_{\alpha 0} \\ D_{0\beta} &= hk^{\beta+1}d_{0\beta} \\ D_{\alpha\beta} &= h^{\alpha+1}k^{\beta+1}d_{\alpha\beta}. \end{aligned} \tag{4.1.10}$$

Finally, for unequal positive integers α, β we define

$$\begin{aligned} E_{\alpha 0} &= E_{0\alpha} = D_{\alpha 0} + D_{0\alpha} \\ E_{\alpha\beta} &= E_{\beta\alpha} = D_{\alpha\beta} + D_{\beta\alpha} \\ E_{\alpha\alpha} &= D_{\alpha\alpha} \end{aligned} \tag{4.1.11}$$

and

$$\begin{aligned} L_{\alpha 0} &= L_{0\alpha} = I_{\alpha 0} + I_{0\alpha} \\ L_{\alpha\beta} &= L_{\beta\alpha} = I_{2s,\beta} + I_{\alpha,2s} \\ L_{\alpha\alpha} &= I_{\alpha\alpha}. \end{aligned} \tag{4.1.12}$$

Theorem 4.1.1 (EULER-MACLAURIN SUMMATION FORMULA)

Let $f \in C^{2s}[R]$. Then

$$I(f) = T(h,k) + \Phi(h,k;2s,2s) + R(h,k;2s,2s) \tag{4.1.13}$$

where

$$\Phi(h,k;2s,2s) = \sum_{\alpha=1}^{s} b_{2\alpha}\left[-E_{2\alpha-1,0} + \sum_{\beta=1}^{\alpha} b_{2\beta}E_{2\alpha-1,2\beta-1}\right] \tag{4.1.14}$$

and

$$R(h,k;2s,2s) = L_{2s,0} - \sum_{\alpha=1}^{s} b_{2\alpha}L_{2s,2\alpha-1} + L_{2s,2s}. \tag{4.1.15}$$

Lyness and McHugh [32] give an n-dimensional formulation of the Euler-Maclaurin Summation formula.

It may be the case for some functions that over the rectangle R, higher partial derivatives exist with respect to the second variable than exist with respect to the first. In this connection we observe that the Euler-Maclaurin Summation formula may be generalized as follows.

Let $C^{2s,2r}[R]$ denote the set of all functions $f(x,y)$ where the partial derivatives $f^{\alpha\beta}$, $0 \leqslant \alpha \leqslant s$, $0 \leqslant \beta \leqslant r$ exist and are continuous on the rectangle R. Then

Theorem 4.1.2

If $f \in C^{2s,2r}[R]$ and $0 \leqslant s < r$, then

$$I(f) = T(h,k) + \Phi(h,k;2s,2r) + R(h,k;2s,2r) \tag{4.1.16}$$

where

$$\begin{aligned} \Phi(h,k;2s,2r) = & \sum_{\alpha=1}^{s} b_{2\alpha}\left[-E_{2\alpha-1,0} + \sum_{\beta=1}^{\alpha} b_{2\beta}E_{2\alpha-1,2\beta-1}\right] \\ & + \sum_{\alpha=s+1}^{r} b_{2\alpha}\left[-D_{0,2\alpha-1} + \sum_{\beta=1}^{s} b_{2\beta}D_{2\beta-1,2\alpha-1}\right] \end{aligned} \tag{4.1.17}$$

and

$$R(h,k;2s,2r) = I_{2s,0} + I_{0,2r} - \sum_{\alpha=1}^{s} b_{2\alpha}(I_{2s,2\alpha-1} + I_{2\alpha-1,2r}) + I_{2s,2s}. \tag{4.1.18}$$

4.2 ERROR ESTIMATES

Let

$$M_{\alpha,\beta} = \max_{(x,y)\in R} |f^{\alpha\beta}(x,y)|$$

$$N_{2s,\alpha} = \begin{cases} h^{2s}k^{\alpha}M_{2s,\alpha} + h^{\alpha}k^{2s}M_{\alpha,2s} & \alpha < 2s \\ 0.74(hk/2\pi)^{2s}M_{2s,2s} & \alpha = 2s \end{cases} \tag{4.2.1}$$

$$0.74 \approx \pi^2/6\sqrt{5}$$

$$1.48 \approx \pi^2/3\sqrt{5}$$

$$2.95 \approx 2\pi^2/3\sqrt{5}$$

$$\gamma = (b-a)(d-c).$$

We now give an estimate for the remainder term in the Euler-Maclaurin Summation formula.

Theorem 4.2.1

Let $f \in C^{2s}[R]$ and

$$P_{2s} = |b_1| N_{2s,0} + \sum_{a=1}^{s} |b_{2a}| N_{2s,2a-1} + N_{2s,2s}. \tag{4.2.2}$$

Then

$$|R(h,k;2s,2s)| \leqslant 2.95(b-a)(d-c)P_{2s}(2\pi)^{-2s}. \tag{4.2.3}$$

Proof:

For $0 \leqslant \alpha \neq \beta \leqslant 2s$ we have

$$|F^{\alpha\beta}(t,u)| \leqslant h^{\alpha+1}k^{\beta+1} \sum_{j=0}^{m-1} \sum_{i=0}^{n-1} |f^{\alpha\beta}(x_i + th, y_j + uk)| \leqslant \gamma h^{\alpha}k^{\beta}M_{\alpha,\beta}. \tag{4.2.4}$$

Take absolute values in (4.1.8) and apply (2.3.1) to obtain the inequality

$$|I_{\alpha\beta}| \leqslant 2.95\,\gamma\lambda h^{\alpha}k^{\beta}M_{\alpha\beta}(2\pi)^{-2s}, \quad \alpha = 2s \quad \text{or} \quad \beta = 2s \tag{4.2.5}$$

where $\lambda = 1/2$ if α or $\beta = 0$ and $\lambda = 1$ otherwise. We estimate $I_{2s,2s}$ as follows.

$$|I_{2s,2s}| \leqslant 1.48^2\gamma(hk)^{2s}M_{2s,2s}(2\pi)^{-4s}. \tag{4.2.6}$$

Finally from (4.1.12) we obtain the result

$$\begin{aligned} |R(h,k,2s,2s)| &\leqslant |L_{2s,0}| + \sum_{a=1}^{s} |b_{2a}L_{2s,2a-1}| + |L_{2s,2s}| \\ &\leqslant 2.95\,\gamma(2\pi)^{-2s}[\,|b_1|N_{2s,0} + \sum_{a=1}^{s} |b_{2a}|N_{2s,2a-1} + N_{2s,2s}] \\ &= 2.95\,\gamma P_{2s}(2\pi)^{-2s} \quad \square \end{aligned} \tag{4.2.7}$$

Theorem 4.2.2

If there exists a positive constant C such that for $0 \leqslant \alpha \leqslant 2s$, $0 < k \leqslant h \leqslant \pi/2$, $M_{2s,\alpha} \leqslant C$, and $M_{\alpha,2s} \leqslant C$, then

$$|R(h,k;2s,2s)| \leqslant 5.93(b-a)(d-c)C(h/2\pi)^{2s}. \tag{4.2.8}$$

The obvious result holds if $0 < h \leqslant k < \pi/2$. Here 5.93 is a bound for the expression

$$\frac{4\pi^2}{3\sqrt{5}}\left[\frac{1}{2} + \frac{\pi^2}{12\sqrt{5}} + \frac{h/12}{1-(h/2\pi)^2}\right] \tag{4.2.9}$$

The proof of this and several succeeding theorems are similar to the proof of Theorem 4.2.3 and therefore are omitted.

Theorem 4.2.3

If there exists a positive constant C such that for $0 < a \leqslant 2s$, $0 < k < h \leqslant \pi/c$, $M_{2s,a} \leqslant C^{2s+a}$, and $M_{a,2s} \leqslant C^{2s+a}$, then

$$|R(h,k;2s,2s)| \leqslant 7.17\,(b-a)(d-c)\left(\frac{hC}{2\pi}\right)^{2s} \tag{4.2.10}$$

Proof:

Apply the bounds on the partial derivatives and the well-known result

$$|b_{2a}| < \frac{2(2\pi)^{-2a}}{1-2^{1-2a}} \tag{4.2.11}$$

to (4.2.7) to obtain

$$\begin{aligned} |R(h,k;2s,2s)| &\leqslant \frac{4\pi^2}{3\sqrt{5}}\gamma\left(\frac{hC}{2\pi}\right)^{2s}\left[\frac{1}{2} + \sum_{a=1}^{s}\frac{\pi^2(hC)^{2a-1}}{3(2\pi)^{2a}} + \frac{\pi^2}{12\sqrt{5}}\left(\frac{hC}{2\pi}\right)^{2s}\right] \\ &\leqslant \frac{4\pi^2}{3\sqrt{5}}\gamma\left(\frac{hC}{2\pi}\right)^{2s}\left[\frac{1}{2} + \left(\frac{hC}{12}\right)\frac{1-(hC/2\pi)^{2s}}{1-(hC/2\pi)^2} + \frac{\pi^2}{12\sqrt{5}}\left(\frac{hC}{2\pi}\right)^{2s}\right] \\ &\leqslant \frac{4\pi^2}{3\sqrt{5}}\gamma\left(\frac{hC}{2\pi}\right)^{2s}\left[\frac{1}{2} + \frac{\pi^2}{12\sqrt{5}} + \frac{hC/12}{1-(hC/2\pi)^2}\right] \end{aligned} \tag{4.2.12}$$

Finally since $hC \leqslant \pi$,

$$\begin{aligned} &\frac{4\pi^2}{3\sqrt{5}}\left[\frac{1}{2} + \frac{\pi^2}{12\sqrt{5}} + \frac{hC/12}{1-(hC/2\pi)^2}\right] \\ &\leqslant \frac{4\pi^2}{3\sqrt{5}}\left[\frac{1}{2} + \frac{\pi^2}{12\sqrt{5}} + \frac{\pi}{9}\right] \leqslant 7.17. \quad \square \end{aligned} \tag{4.2.13}$$

4.3 ADDITIONAL ERROR ESTIMATES

For $0 \leqslant \alpha, \beta < 2s$ we note that

$$I_{2s,\beta} = -I_{2s+1,\beta}, \; I_{\alpha,2s} = -I_{\alpha,2s+1}, \; I_{2s,2s} = I_{2s+1,2s+1}. \tag{4.3.1}$$

Hence we have the inequalities:

$$\begin{aligned} |I_{2s+1,\beta}| &\leqslant 2.95\,\gamma\lambda h^{2s+1}k^{\beta}M_{2s+1,\beta}(2\pi)^{-(2s+1)} \\ |I_{\alpha,2s+1}| &\leqslant 2.95\,\gamma\lambda h^{\alpha}k^{2s+1}M_{\alpha,2s+1}(2\pi)^{-(2s+1)} \\ |I_{2s,2s}| &\leqslant 1.48^2\,\gamma(hk)^{2s+1}M_{2s+1,2s+1}(2\pi)^{-(4s+2)} \end{aligned} \tag{4.3.2}$$

where $\lambda = 1/2$ if α or β is zero and $\lambda = 1$ otherwise. Then the analog of Theorem 4.2.1 is

Theorem 4.3.1

$$\begin{aligned} |R(h,k;2s,2s)| &= |R(h,k;2s+1,2s+1)| \\ &\leqslant 2.95(b-a)(d-c)P_{2s+1}(2\pi)^{-(2s+1)} \end{aligned} \tag{4.3.3}$$

where

$$P_{2s+1} = |b_1|N_{2s+1,0} + \sum_{\alpha=1}^{s} |b_{2\alpha}|N_{2s+1,2\alpha-1} + N_{2s+1,2s+1}. \tag{4.3.4}$$

$$N_{2s+1,2s+1} = \frac{\pi^2}{6\sqrt{5}}\left(\frac{hk}{2\pi}\right)^{2s} M_{2s+1,2s+1}.$$

Theorem 4.3.2

Theorem 4.2.2 is true if $2s$ is replaced by $2s + 1$.

Theorem 4.3.3

Theorem 4.2.3 holds if $2s$ is replaced by $2s + 1$.

4.4 SHARPER ERROR ESTIMATES

Due to the asymptotic nature of the Euler-Maclaurin series, the following error estimates will often provide closer error estimates than those given in the two previous sections.

Theorem 4.4.1

$$|R(h,k;2s{+}1,2s{+}1)| \leqslant 5.31(b-a)(d-c)P_{2s+2}(2\pi)^{-(2s+2)} \tag{4.4.1}$$

where

$$P_{2s+2} = |b_1|N_{2s+2,0} + \sum_{a=1}^{s} |b_{2a}|N_{2s+2,2a-1} + N_{2s+2,2s+2}.$$

$$N_{2s+2,2s+2} = \left(\frac{hk}{2\pi}\right)^{2s} \frac{M_{2s+1,2s+1}}{\sqrt{6}}, \tag{4.4.2}$$

and

$$5.31 \approx \pi^4\sqrt{6}/45.$$

Proof:

Recall from (2.1.2), (2.1.7), (2.1.8), and (2.1.10) the following properties:

$$\begin{aligned} &\phi_\beta(1) = \phi_\beta(0), \quad \beta > 1 \\ &\int_0^1 \phi_\beta^2(t)dt = (-1)^{\beta+1}b_{2\beta} \leqslant 2.17(2\pi)^{-2\beta} \\ &|b_{4\beta}| \leqslant \frac{1}{2}b_{2\beta}^2 \\ &2.17 \approx \pi^4/45. \end{aligned} \tag{4.4.3}$$

For convenience we let $\pm$ signify $+$ if $\beta = 0$ and $-$ if $\beta > 0$. Also, let $\mp$ signify $-$ if $\beta = 0$ and $+$ if $\beta > 0$. Then integrating by parts and applying (4.4.3) we find

$$\begin{aligned} -I_{2s,\beta} &= -\int_0^1 [F^{2s,\beta}(t,1) \pm F^{2s,\beta}(t,0)]\,\phi'_{2s+1}(t)dt \\ &= \mp b_{2s+1}D_{2s,\beta} + I_{2s+1,\beta} \\ &= I_{2s+1,\beta} \\ &= \pm b_{2s+2}D_{2s+1,\beta} - I_{2s+2,\beta} \\ &= \int_0^1 [F^{2s+2,\beta}(t,1) \pm F^{2s+2,\beta}(t,0)]\,[\pm b_{2s+2} - \phi_{2s+2}(t)]\,dt. \end{aligned} \tag{4.4.4}$$

Apply the Cauchy-Schwarz inequality and use (4.4.3) to obtain

$$|I_{2s+1,\beta}| \leqslant 2\gamma h^{2s+2}k^{\beta}M_{2s+2,\beta}(b_{2s+2}^2 - b_{4s+4})^{1/2}$$
$$\leqslant 5.31\gamma h^{2s+2}k^{\beta}M_{2s+2,\beta}(2\pi)^{-(2s+2)}. \tag{4.4.5}$$

Similarly

$$-I_{a,2s} = I_{a,2s+1}$$
$$|I_{a,2s+1}| \leqslant 5.31\gamma h^{a}k^{2s+2}M_{a,2s+2}(2\pi)^{-(2s+2)}. \tag{4.4.6}$$

Moreover

$$I_{2s,2s} = I_{2s+1,2s+1}. \tag{4.4.7}$$

Applying these results to (4.1.15) we have

$$R(h,k;2s,2s) = -R(h,k;2s+1,2s+1)$$
$$= -L_{2s+1,0} + \sum_{a=1}^{s} b_{2a}L_{2s+1,2a-1} - L_{2s+1,2s+1}. \tag{4.4.8}$$

Finally

$$|R(h,k;2s,2s)| = |R(h,k;2s+1,2s+1)|$$
$$\leqslant 5.31\gamma(2\pi)^{-(2s+2)}[|b_1|N_{2s+2,0}$$
$$+ \sum_{a=1}^{s} |b_{2a}|N_{2s+2,2a-1} + N_{2s+2,2s+2}]. \;\square \tag{4.4.9}$$

Theorem 4.4.2

If there exists a constant C such that for $0 \leqslant a \leqslant 2s$, $0 < k \leqslant h \leqslant \pi$, $M_{2s+2,a} \leqslant C$, and $M_{a,2s+2} \leqslant C$ then

$$|R(h,k;2s,2s)| \leqslant 11.17(b-a)(d-c)C(h/2\pi)^{2s+2}. \tag{4.4.10}$$

Here 11.17 approximates

$$\frac{\pi^4\sqrt{6}}{45}\left[1 + 6^{-1/2} + \frac{h/6}{1-(h/2\pi)^2}\right]. \tag{4.4.11}$$

Theorem 4.4.3

If there is a constant C such that for $0 \leqslant a \leqslant 2s$, $0 < k \leqslant h \leqslant \pi/C$, $M_{2s+2,a} \leqslant C^{2s+a}$, and $M_{a,2s+2} \leqslant C^{2s+a}$, then

$$|R(h,k;2s,2s)| = |R(h,k;2s{+}1,2s{+}1)|$$

$$\leqslant 10.61\ (b-a)(d-c)\left(\frac{hC}{2\pi}\right)^{2s+2}\left[\frac{6+\sqrt{6}}{12} + \frac{hC/12}{1-(hC/2\pi)^2}\right] \tag{4.4.12}$$

where

$$10.61 \approx 2\pi^4\sqrt{6}/45. \tag{4.4.13}$$

Proof:

$$|R(h,k;2s{+}1,2s{+}1)|$$

$$\leqslant \frac{\pi^4\sqrt{6}}{45}(b-a)(d-c)\left(\frac{h}{2\pi}\right)^{2s+2} 2C^{2s+2}\left[|b_1| + \sum_{a=1}^{s}|b_{2a}|(hC)^{2a-1} + \left(\frac{hC}{2\pi}\right)^{2s}\frac{1}{2\sqrt{6}}\right]$$

$$\leqslant \frac{2\pi^4\sqrt{6}}{45}(b-a)(d-c)\left(\frac{hC}{2\pi}\right)^{2s+2}\left[\frac{1}{2} + \sum_{a=1}^{s}\frac{\pi^2}{3}(2\pi)^{-2a}(hC)^{2a-1} + \frac{\sqrt{6}}{12}\right] \tag{4.4.14}$$

$$\leqslant \frac{2\pi^4\sqrt{6}}{45}(b-a)(d-c)\left(\frac{hC}{2\pi}\right)^{2s+2}\left[\frac{6+\sqrt{6}}{12} + \frac{\pi}{6}\left(\frac{hC}{2\pi}\right)\frac{1-(hC/2\pi)^{2s}}{1-(hC/2\pi)^2}\right]. \quad \square$$

4.5 A NUMERICAL EXAMPLE

The Euler-Maclaurin Summation Formula (4.1.13) applied to the integral

$$I(f) = \int_0^1\int_0^1 \frac{dxdy}{x+y+1} = \ln(27/16) = 0.523\ 248\ 144 \tag{4.5.1}$$

results in the formulation

$$I(f) - R(h,h;2s,2s) = \Phi(h,h;2s,2s)$$

$$\begin{aligned} &= h^2 \sum_{j=0}^{n}{}'' \sum_{i=0}^{n}{}'' \frac{1}{(i+j)h+1} \\ &- \sum_{a=1}^{s} b_{2a}h^{2a}\Bigg[2h(2a-1)!\sum_{\beta=0}^{n}{}''\left\{(1+\beta h)^{-2a} - (2+\beta h)^{-2a}\right\} \\ &+ \sum_{\beta=1}^{a-1} 2b_{2\beta}h^{2\beta}(2a+2\beta-2)!\left\{4^{1-(a+\beta)} - 3^{1-2(a+\beta)} - 1\right\} \\ &+ b_{2a}h^{2a}(4a-2)!\left\{4^{1-2a} - 3^{1-4a} - 1\right\}\Bigg] \end{aligned} \tag{4.5.2}$$

where

$$h = \frac{1}{n}, \quad n = 1, 2, \cdots$$

$$f^{\alpha\beta}(x,y) = \frac{(-1)^{\alpha+\beta}(\alpha+\beta)!}{(x+y+1)^{\alpha+\beta+1}}. \tag{4.5.3}$$

Applying the error estimates (4.2.3), (4.3.3), and (4.4.1) we find

$$|R(h,h;2s,2s)| \leqslant 2.95\left(\frac{h}{2\pi}\right)^{2s}\left[(2s)! + 2\sum_{\alpha=1}^{s} |b_{2\alpha}| h^{2\alpha-1}(2s+2\alpha-1)! + .74\left(\frac{h}{2\pi}\right)^{2s}(4s)!\right] \tag{4.5.4}$$

$$|R(h,h;2s,2s)| \leqslant 2.95\left(\frac{h}{2\pi}\right)^{2s+1}\left[(2s+1)! + 2\sum_{\alpha=1}^{s} |b_{2\alpha}| h^{2\alpha-1}(2s+2\alpha)! + .74\left(\frac{h}{2\pi}\right)^{2s+1}(4s+2)!\right] \tag{4.5.5}$$

$$|R(h,h;2s+1,2s+1)| \leqslant 5.31\left(\frac{h}{2\pi}\right)^{2s+2}\left[(2s+2)! + 2\sum_{\alpha=1}^{s} |b_{2\alpha}|(2s+2\alpha+1)! + \frac{1}{\sqrt{6}}\left(\frac{h}{2\pi}\right)^{2s}(4s+2)!\right] \tag{4.5.6}$$

The results are presented in Tables 4.5.1–4.5.7. The partial derivative correction sums are given in Table 4.5.1. Table 4.5.2 gives the results of the Euler-Maclaurin Summation formula for several values of h and s; the associated errors are listed in Table 4.5.3.

Tables 4.5.4 through 4.5.6 present the results of applying the error estimates (4.5.4) through (4.5.6), respectively. Finally, in Table 4.5.7, we give the absolute value of the ratio (Error Estimate 4.5.k)/(Actual Error), $k = 4, 5, 6$. The results indicate that the choice of the error estimate depends not only on the integrand f but also on the values of h and s.

For values of $s \ll 1/h$, (4.5.6) provides the sharpest error estimate while for $s \gg 1/h$, (4.5.4) should be used. For $s \approx 1/h$, (4.5.5) provides the best estimate of the truncation error.

In practice, one would fix the value of s and let h decrease to zero. In this case, error estimate (4.5.6) should be applied.

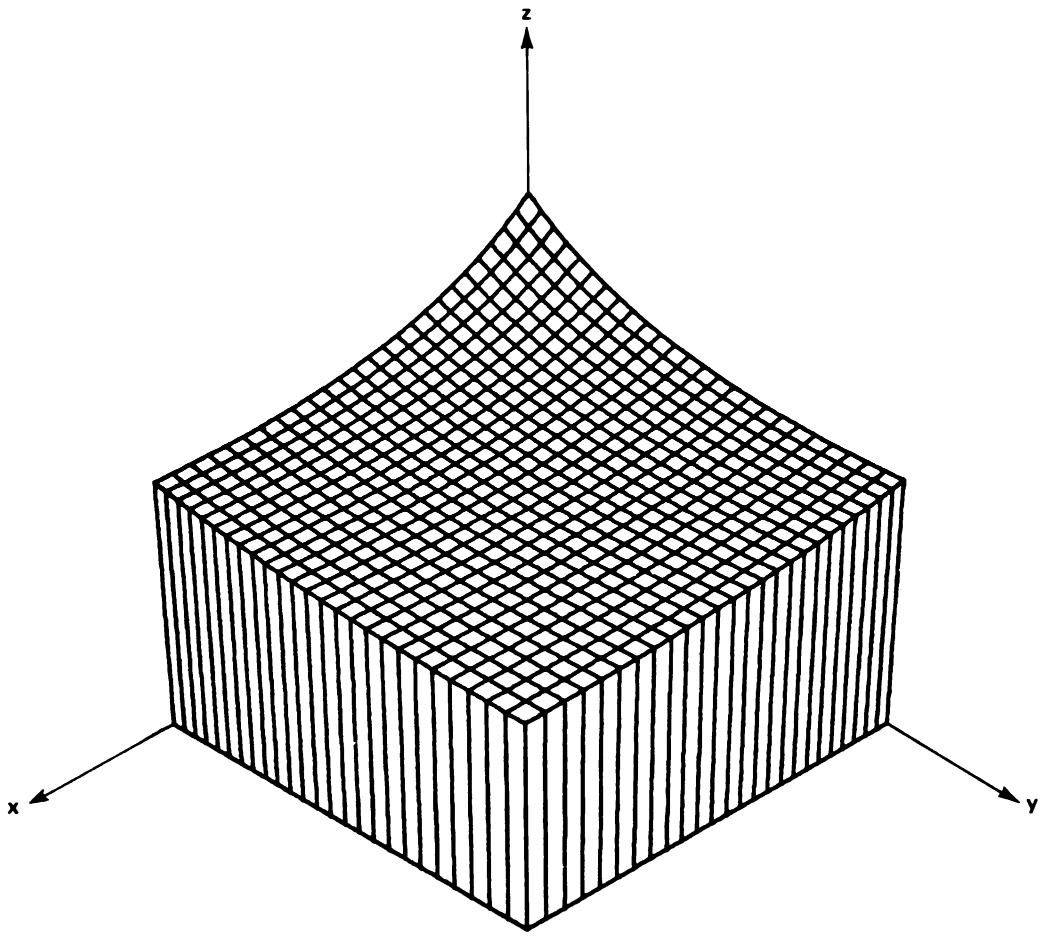


Figure 4.5.1 Graph of $z = (x + y + 1)^{-1}$ on $[0,1]^2$

Table 4.5.1 Partial Derivative Correction Sums $\Phi(h,h;2s,2s)$

h \ s	1	2	3	4	5
1	.063 143 004	.058 775 925	.058 555 694	.018 202 954	-2.147 609 63
1/2	.014 501 993	.014 231 639	.014 255 757	.014 250 457	.014 251 156
1/3	.006 301 135	.006 247 312	.006 249 366	.006 249 187	.006 249 216
1/4	.003 513 700	.003 496 638	.003 497 003	.003 496 985	
1/5	002 239 387	.002 232 394	.002 232 490		
1/10	.005 566 435	.005 562 062			

Table 4.5.2 Euler-Maclaurin Summation Formula: $I(f) = 0.523\ 248\ 144 \approx T(h,h) - \Phi(h,h;2s,2s)$

h \ s	0	1	2	3	4	5
1	.583 333 333	.520 190 329	.524 557 409	.524 777 640	.565 130 379	2.730 942 96
1/2	.537 500 000	.522 998 007	.523 268 361	.523 244 843	.523 249 543	.523 248 844
1/3	.529 497 354	.523 196 230	.523 250 043	.523 247 989	.523 248 167	.523 248 138
1/4	.526 745 130	.523 231 430	.523 248 492	.523 248 127	.523 248 145	
1/5	.525 480 630	.523 241 243	.523 248 236	.523 248 140		
1/10	.523 804 351	.523 247 708	.523 248 146			

Table 4.5.3 Error $R(h,h;2s,2s) = I(f) - T(h,h) + \Phi(h,h;2s,2s)$

h \ s	0	1	2	3	4	5
1	-6.01-2*	3.06-3	-1.31-3	-1.53-3	-4.19-2	-2.21+0
1/2	-1.43-2	2.50-4	-2.02-5	3.30-6	-1.40-6	-7.00-7
1/3	-6.25-3	5.19-5	-1.90-6	1.55-7	-2.32-8	5.20-9
1/4	-3.50-3	1.67-5	-3.49-7	1.65-8	-1.40-9	
1/5	-2.23-3	6.90-6	-9.24-8	3.30-9		
1/10	-5.56-4	4.35-7	-1.80-9			

*-6.01-2 means -6.01×10^{-2}.

Table 4.5.4 Estimates for $R(h,h;2s,2s)$ using (4.5.4)

h \ s	1	2	3	4	5
1	2.57–1	1.45–1	5.23–1	1.11+1	7.50+2
1/2	4.87–2	4.36–3	1.07–3	6.57–4	1.34–3
1/3	1.97–2	7.32–4	6.93–5	1.26–5	3.99–6
1/4	1.06–2	2.16–4	1.11–5	1.07–6	1.67–7
1/5	6.61–3	8.50–5	2.75–6	1.66–7	1.61–8
1/10	1.57–3	4.91–6	3.85–8	5.63–10	1.32–11

Table 4.5.5 Estimates for $R(h,h;2s,2s)$ using (4.5.5)

h \ s	1	2	3	4	5
1	1.44–1	1.88–1	1.67+0	6.77+1	7.26+3
1/2	1.23–2	1.90–3	7.10–4	7.10–4	2.63–3
1/3	3.26–3	2.04–4	2.74–5	6.55–6	2.73–6
1/4	1.30–3	4.46–5	3.21–6	4.00–7	7.73–8
1/5	6.47–4	1.39–5	6.31–7	4.91–8	5.85–9
1/10	7.59–5	3.97–7	4.36–9	8.19–11	2.35–12

Table 4.5.6 Estimates for $R(h,h;2s,2s)$ using (4.5.6)

h \ s	1	2	3	4	5
1	1.75–1	3.03–1	2.62+0	9.83+1	1.00+4
1/2	7.63–3	1.78–3	9.07–4	1.11–3	4.31–3
1/3	1.32–3	1.24–4	2.23–5	6.81–6	3.53–6
1/4	3.92–4	2.00–5	1.92–6	3.01–7	7.04–8
1/5	1.54–4	4.95–6	2.99–7	2.91–8	4.17–9
1/10	8.87–6	6.94–8	1.01–9	2.38–11	8.22–13

Table 4.5.7 |(Error Estimate 4.3.k)/Error|, k = 4,5,6

h \ s	1	2	3	4	5
1	84 47 57	111 144 231	342 1092 1712	265 1616 2346	339 3284 4575
1/2	195 49 31	216 94 88	324 215 275	469 507 793	1914 3757 6157
1/3	380 63 25	385 107 65	447 177 144	543 282 294	767 525 679
1/4	635 78 23	619 128 57	673 195 116	764 286 215	835 387 352
1/5	958 94 22	920 150 54	833 191 91		
1/10	3609 174 20	2728 221 39			

5. APPLICATIONS OF THE 2-DIMENSIONAL EULER-MACLAURIN SUMMATION FORMULA

5.1 CUBATURE FORMULAS WITH ASYMPTOTIC EXPANSIONS

The generalization of the quadrature formulas in Section 3.1 to functions of two variables involves expressing the Euler-Maclaurin Summation formula (4.1.15) in terms of a rectangular grid and taking appropriate weighted trapezoidal sums for various grid sizes in order to eliminate the desired number of terms in the asymptotic error expansion. The result is a cubature formula of the required degree of precision. The details of the technique are as follows.

Let $1 \leqslant a_1 < a_2 < \cdots < a_{s+1}$ be factors of $n = (b-a)/h$ and $m = (d-c)/k$. For $1 \leqslant i$, $j \leqslant s+1$, define the $\eta + 1 = (s+1)(s+2)/2$ trapezoidal sums

$$T_{ij} = \lambda_{ij}[T(a_i h, a_j k) + T(a_j h, a_i k)] \tag{5.1.1}$$

where

$$\lambda_{ij} = \begin{cases} 1/2 \text{ if } i = j \\ 1 \text{ otherwise} \end{cases} \tag{5.1.2}$$

and $T(h,k)$ is defined by (4.1.4). For convenience, we define $E_{\beta,-1} = E_{\beta 0}$ and $E_{-1,\beta} = E_{0\beta}$.

Denote by

$$A = A^{(a_1,a_1)(a_2,a_1)\cdots(a_s,a_1)(a_2,a_2)\cdots(a_s,a_s)}_{(2\beta_{11}-1,2\beta_{12}-1)(2\beta_{21}-1,2\beta_{22}-1)\cdots(2\beta_{n1}-1,2\beta_{n2}-1)}(h,k) \tag{5.1.3}$$

the approximation to the double integral

$$I(f) = \int_c^d \int_a^b f(x,y)dxdy \tag{5.1.4}$$

based on the weighted average of the η sums $T_{a_i a_j}$, $1 \leqslant i$, $j \leqslant s+1$ which eliminates the η terms involving $E_{2\beta_{i1}-1,\,2\beta_{i2}-1}$, $1 \leqslant i \leqslant \eta$, but possibly has some lower-order partial derivative correction terms, $E_{2\gamma_{i1}-1,\,2\gamma_{i2}-1}$, $1 \leqslant i \leqslant t$.

Let

$$\delta_{ij} = \begin{cases} 1 & \text{if } \beta_{ij} = 0 \\ 2\beta_{ij} & \text{otherwise} \end{cases} \tag{5.1.5}$$

and

$$C_{j_1 j_2}^{i_1 i_2} = \lambda_{j_1 j_2}\left[a_{j_1}^{\delta_{i_1 1}} a_{j_2}^{\delta_{i_2 2}} + a_{j_2}^{\delta_{i_1 1}} a_{j_1}^{\delta_{i_2 2}}\right]. \tag{5.1.6}$$

We wish to find $\eta + 1$ constants x_{ij} such that

$$A = \sum_{i \geq j = 1}^{n+1} x_{ij} T_{a_i a_j} = I(f) + C b_{2u} b_{2v} Q_{2u-1,2v-1} \tag{5.1.7}$$

where C is some constant, u and v are appropriate nonnegative integers, and Q is given by

$$Q_{2u-1,2v-1} = \sum_{i \geq j = 1}^{n+1} x_{ij} E_{2u-1,2v-1}(a_i h, a_j k). \tag{5.1.8}$$

If we write $w_1 = x_{11}$, $w_2 = x_{21}, \cdots, w_{\eta+1} = x_{s+1,s+1}$, then the $\eta+1$ constants w_i may possibly be found by solving the linear system

$$\begin{bmatrix} 2\lambda_{11} & 2\lambda_{21} & \cdots & 2\lambda_{s1} & 2\lambda_{22} & \cdots & 2\lambda_{s2} & \cdots & 2\lambda_{s+1,s+1} \\ C_{11}^{11} & C_{21}^{11} & \cdots & C_{s1}^{11} & C_{22}^{11} & \cdots & C_{s2}^{11} & \cdots & C_{s+1,s+1}^{11} \\ C_{11}^{22} & C_{21}^{22} & \cdots & C_{s1}^{22} & C_{22}^{22} & \cdots & C_{s2}^{22} & \cdots & C_{s+1,s+1}^{22} \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & & \vdots \\ C_{11}^{\eta\eta} & C_{21}^{\eta\eta} & \cdots & C_{s1}^{\eta\eta} & C_{22}^{\eta\eta} & \cdots & C_{s2}^{\eta\eta} & \cdots & C_{s+1,s+1}^{\eta\eta} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_{\eta+1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{5.1.9}$$

If a solution to (5.1.9) exists, then for some integer σ we obtain an asymptotic expansion for the cubature formula, A:

$$\begin{aligned} A &= \sum_{i \geq j = 1}^{s+1} x_{ij} T_{a_i a_j} - \sum_{l=1}^{t} b_{2\gamma_{l1}} b_{2\gamma_{l2}} Q_{2\gamma_{l1}-1,2\gamma_{l2}-1} \\ &= I(f) + \Omega(h,k;\sigma\sigma). \end{aligned} \tag{5.1.10}$$

Note that in some cases, for example, $A^{(1,1)(2,1)(2,2)(4,1)(4,2)(4,4)}_{(1,0)(3,0)(3,1)(3,3)(5,0)}(h,k)$, correction terms of the form E_{a0} may not be eliminated.

Recalling (4.1.15), the definition of $R(h, k; 2s, 2s)$, we write

$$R_{a_i a_j} = \lambda_{ij}[R(a_i h, a_j k; \sigma, \sigma) + R(a_j h, a_i k; \sigma, \sigma)]. \tag{5.1.11}$$

Then the truncation error Ω in (5.1.10) is

$$\Omega(h,k;\sigma,\sigma) \mp \sum_{i>j=1}^{s} x_{ij} R_{a_i a_j} \tag{5.1.12}$$

and may be estimated by the methods of Chapter 4.

To illustrate the technique we will derive the partial derivative corrected (DC) Simpson rule:

$$S'(h,k) = A_{(3,0)(3,1)}^{(1,1)(2,1)(2,2)}(h,k). \tag{5.1.13}$$

Setting $s = 1$, $\eta = 2$, $(a_1, a_1) = (1,1)$, $(a_2, a_1) = (2,1)$, $(a_2, a_2) = (2,2)$, $(\beta_{11}, \beta_{12}) = (2,0)$, $(\beta_{21,22}) = (2,1)$, $(\gamma_{11}, \gamma_{12}) = (1,0)$, and $(\gamma_{21}, \gamma_{22}) = (1,1)$ we obtain the system

$$\begin{bmatrix} 1 & 2 & 1 \\ 1 & 18 & 32 \\ 1 & 20 & 64 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{5.1.14}$$

having the unique solution

$$(w_1, w_2, w_3) = (256/225, -16/225, 1/225). \tag{5.1.15}$$

Thus we obtain (5.2.4), an asymptotic expansion for the DC Simpson's rule. The error is given by

$$\Omega(h,k;2s,2s) = [256\,R_{11} - 16\,R_{21} + R_{22}]/225. \tag{5.1.16}$$

This cubature rule is illustrated in Figure 5.2.5 and the trapezoidal sums are shown in Figure 5.2.4.

In Section 5.2 we give without comment several cubature formulas with asymptotic expansions, error terms, and appropriate diagrams. These formulas are the 2-dimensional generalizations of the quadrature formulas of Section 3.1. Some of the results, e.g., the DC Weddle's rule, are believed to be new. Sheppard [45] obtained the double Simpson's and Weddle's rules. A number of additional cubature rules were obtained but are not presented here.

Using another technique, Tanimoto [50] derived what we call the DC Simpson's rule, (5.2.4). However, his paper has several errors. Moreover, he does not give an expression for the error.

Finally we note that

$$A^{(1,1)(2,1)(2,2)(4,1)(4,2)(4,4)}_{(1,0)(1,1)(3,0)(3,1)(5,1)} \qquad (5.1.17)$$

results in the linear system

$$\begin{bmatrix} 1 & 2 & 1 & 2 & 2 & 1 \\ 1 & 6 & 8 & 20 & 48 & 64 \\ 1 & 8 & 16 & 32 & 128 & 256 \\ 1 & 18 & 32 & 260 & 576 & 1024 \\ 1 & 20 & 64 & 272 & 1280 & 4096 \\ 1 & 68 & 256 & 4112 & 17408 & 65536 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad (5.1.18)$$

in which the coefficient matrix is singular.[1] In this case there are infinitely many solutions.

5.2 SOME CUBATURE FORMULAS OBTAINED FROM THE EULER-MACLAURIN SUMMATION FORMULA

Euler-Maclaurin Summation Formula: Trapezoidal Rule

$$\begin{aligned} T(h,k) &\equiv hk \sum_{j=0}^{m}{}'' \sum_{i=0}^{n}{}'' f(a+ih, c+jk) \\ &= \int_c^d \int_a^b f(x,y)dxdy + \frac{E_{10}}{12} - \frac{E_{11}}{144} \\ &\quad - \frac{E_{30}}{720} - \frac{E_{31}}{8640} - \frac{E_{33}}{518\,400} \\ &\quad + \frac{E_{50}}{30\,240} + \frac{E_{51}}{362\,880} - \frac{E_{53}}{21\,772\,800} - \frac{E_{55}}{914\,457\,600} \\ &\quad - \frac{E_{70}}{1\,209\,600} - \frac{E_{71}}{14\,515\,200} + \frac{E_{73}}{870\,912\,000} - \frac{E_{75}}{36\,578\,304\,000} \end{aligned} \qquad (5.2.1)$$

(Equation (5.2.1) continues)

[1] If the 1 on the right side of (5.1.18) is changed to 2025, then a solution is given by (4096, −1280, 400, 64, −20, 1). This system proved difficult to evaluate numerically. A modified version of the Fortran program recommended by Forsythe and Moler [17] was used.

$$- \frac{E_{77}}{1\,463\,032\,160\,000} + \frac{E_{90}}{47\,900\,160} + \frac{E_{91}}{574\,801\,920} - \frac{E_{93}}{34\,488\,115\,200}$$

$$+ \frac{E_{95}}{1\,448\,500\,838\,400} - \frac{E_{97}}{57\,940\,033\,536\,000} - \frac{E_{99}}{2\,294\,425\,328\,025\,000}$$

$$- \cdots + b_{2s}\left[E_{2s-1,0} + \sum_{\beta=1}^{s} b_{2\beta} E_{2s-1,2\beta-1}\right] + R\,(h,k;2s,2s). \tag{5.2.1}$$

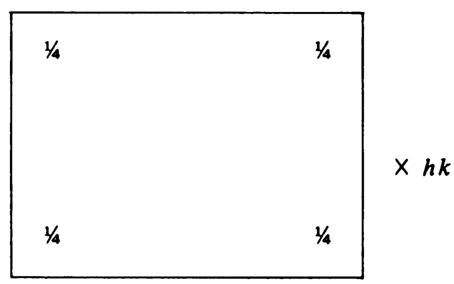


Figure 5.2.1 Trapezoidal Rule

DC Trapezoidal Rule

$$T'(h,k) = T(h,k) - \frac{E_{10}}{12} + \frac{E_{11}}{144}$$

$$= I(f) - \frac{E_{30}}{720} - \frac{E_{31}}{8640} - \frac{E_{33}}{518\,400} + \cdots \tag{5.2.2}$$

$$+ b_{2s}\left[E_{2s-1,0} + \sum_{\beta=1}^{s} b_{2\beta} E_{2s-1,2\beta-1}\right] + R\,(h,k;2s,2s).$$

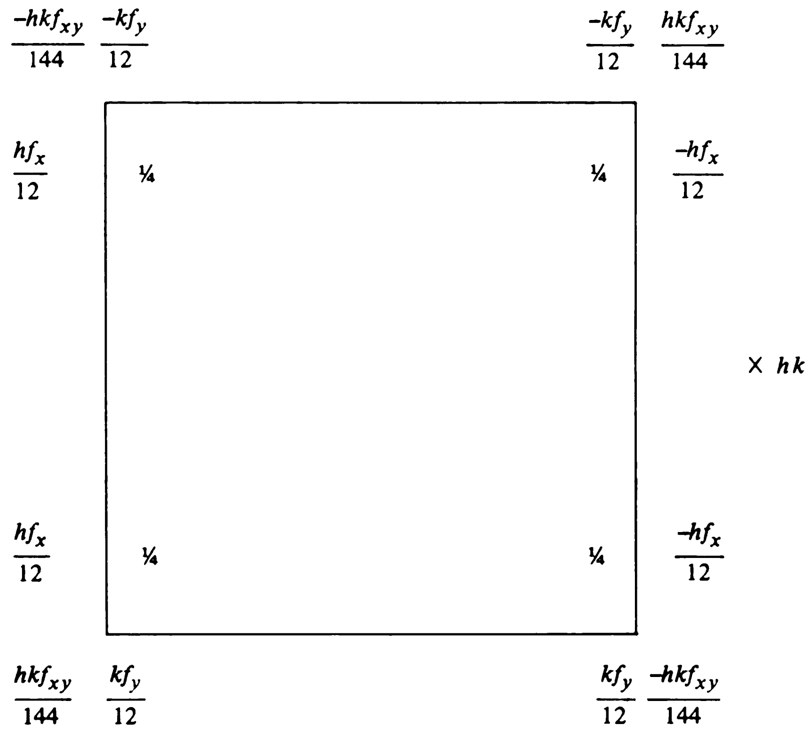


Figure 5.2.2 DC Trapezoidal Rule

Simpson's Rule

$$
\begin{aligned}
S(h,k) &= A^{(1,1)(2,1)(2,2)}_{(1,0)(1,1)}(h,k) \\
&= [16\,T_{11} - 4\,T_{21} + T_{22}]/9 \\
&= I(f) - \frac{Q_{30}}{720} - \frac{E_{33}}{32\,400} + \frac{Q_{50}}{30\,240} - \frac{E_{53}}{272\,160} - \frac{E_{55}}{2\,286\,144} + \cdots \\
&\quad + b_{2s}\left[Q_{2s-1,0} + \frac{1}{9}\sum_{\beta=1}^{s} b_{2\beta}\,[16 - 4(4^s + 4^\beta) + 4^{s+\beta}]\,E_{2s-1,2\beta-1}\right] + \Omega(h,k;2s,2s).
\end{aligned}
\qquad (5.2.3)
$$

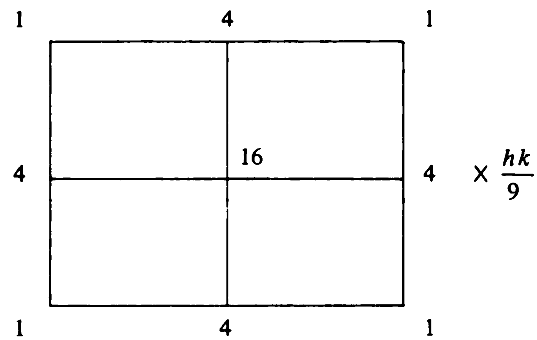


Figure 5.2.3 Simpson's Rule

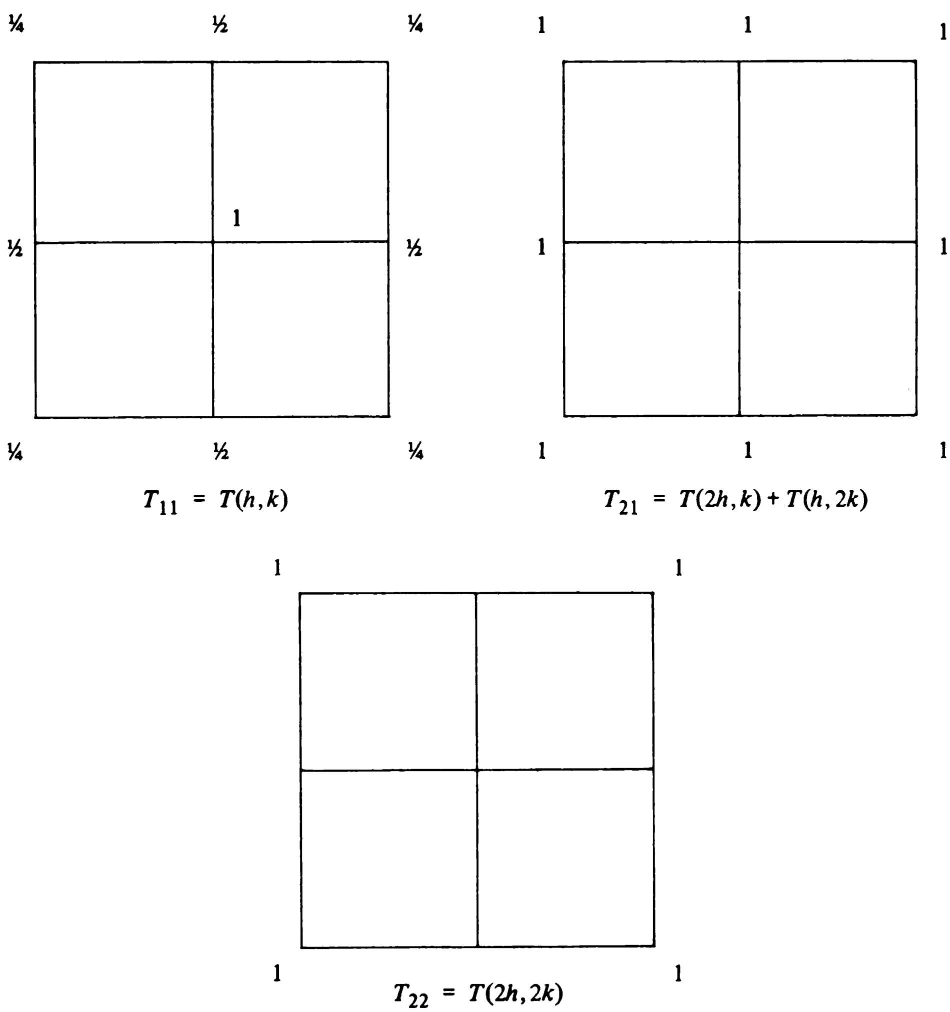


Figure 5.2.4 Component Trapezoidal Sums for Simpson's Rule

DC Simpson's Rule

$$
\begin{aligned}
S'(h,k) &= A^{(1,1)(2,1)(2,2)}_{(3,0)(3,1)}(h,k) \\
&= [256\,T_{11} - 16\,T_{21} + T_{22}]/225 - \frac{Q_{10}}{12} + \frac{E_{11}}{225} \\
&= I(f) + \frac{Q_{50}}{30\,240} - \frac{E_{51}}{141\,750} - \frac{E_{55}}{89\,302\,500} \qquad (5.2.4) \\
&\quad + b_{2s}\left[Q_{2s-1,0} + \frac{1}{225}\sum_{\beta=1}^{s} b_{2\beta}\,[256 - 16(4^s + 4^\beta) + 4^{s+\beta}]\,E_{2s-1,2\beta-1}\right] \\
&\quad + \Omega(h,k;2s,2s).
\end{aligned}
$$

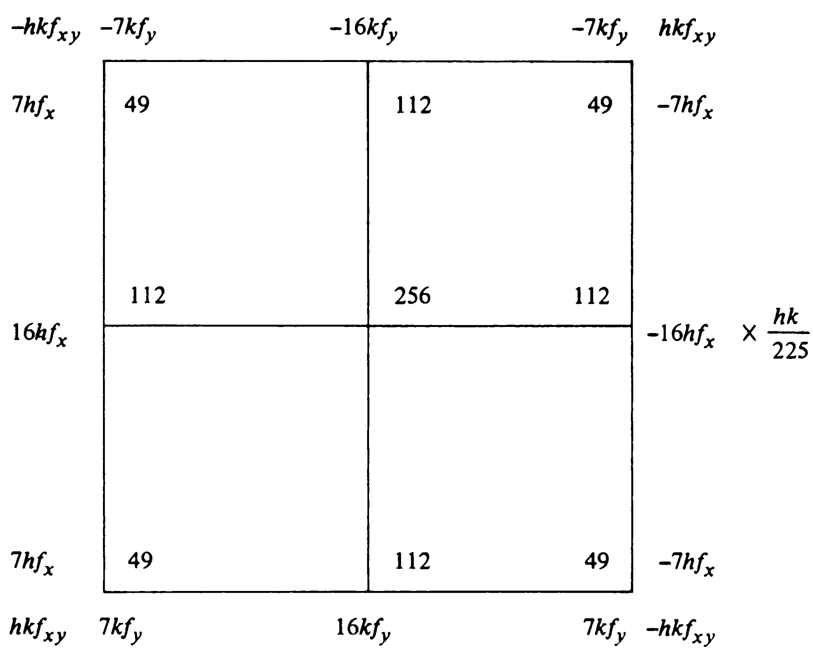


Figure 5.2.5 DC Simpson's Rule

Simpson's Second Rule

$$A^{(1,1)(3,1)(3,3)}_{(1,0)(1,1)}(h,k) = [81\,T_{11} - 9\,T_{31} + T_{33}]/64$$

$$= I(f) - \frac{Q_{30}}{720} - \frac{E_{33}}{6400} + \frac{Q_{50}}{30\,240} - \frac{E_{53}}{26\,880} - \frac{E_{55}}{112\,896} + \cdots$$

$$+ b_{2s}\left[Q_{2s-1,0} + \frac{1}{64}\sum_{\beta=1}^{s} b_{2\beta}\,[81 - 9(9^s + 9^\beta) + 9^{s+\beta}]\,E_{2s-1,2\beta-1}\right] \qquad (5.2.5)$$

$$+ \Omega(h,k;2s,2s).$$

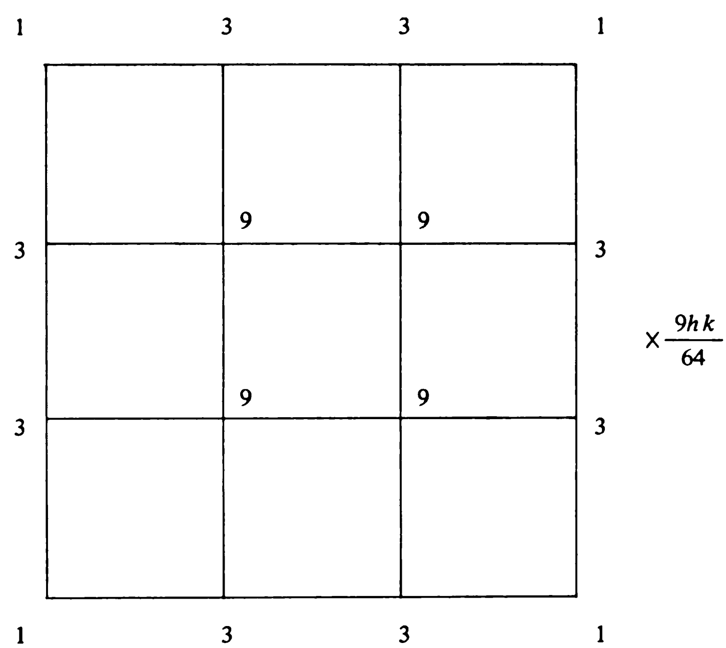
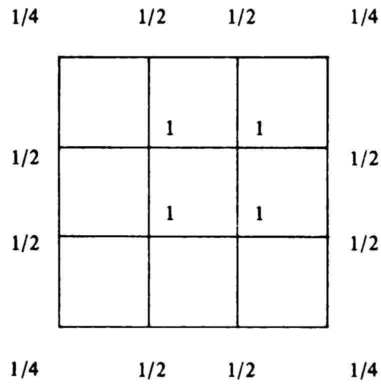
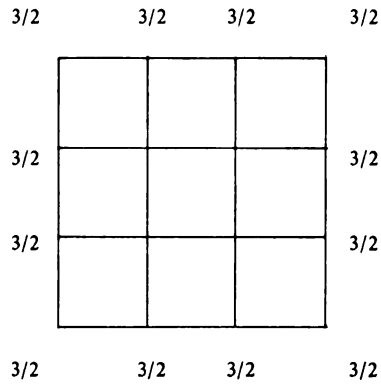


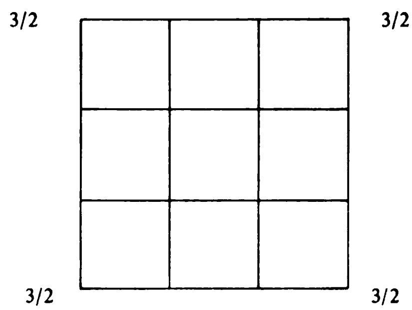
Figure 5.2.6 Simpson's Second Rule



$T_{11} = T(h,k)$



$T_{31} = T(3h,k) + T(h,3k)$



$T_{33} = T(3h,3k)$

Figure 5.2.7 Component Trapezoidal Sums for Simpson's Second Rule

DC Simpson's Second Rule

$$A^{(1,1)(3,1)(3,3)}_{(3,0)(3,1)}(h,k) = [6561\,T_{11} - 81\,T_{31} + T_{33}]/6400 - \frac{Q_{10}}{12} + \frac{9E_{11}}{1600}$$

$$= I(f) + \frac{Q_{50}}{30\,240} - \frac{9E_{51}}{44\,800} - \frac{9E_{55}}{1\,254\,400} + \cdots \qquad (5.2.6)$$

$$+ b_{2s}\left[Q_{2s-1,0} + \frac{1}{6400}\sum_{\beta=1}^{s} b_{2\beta}[6561 - 81(9^s + 9^\beta) + 9^{s+\beta}]\,E_{2s-1,2\beta-1}\right] + \Omega(h,k;2s,2s).$$

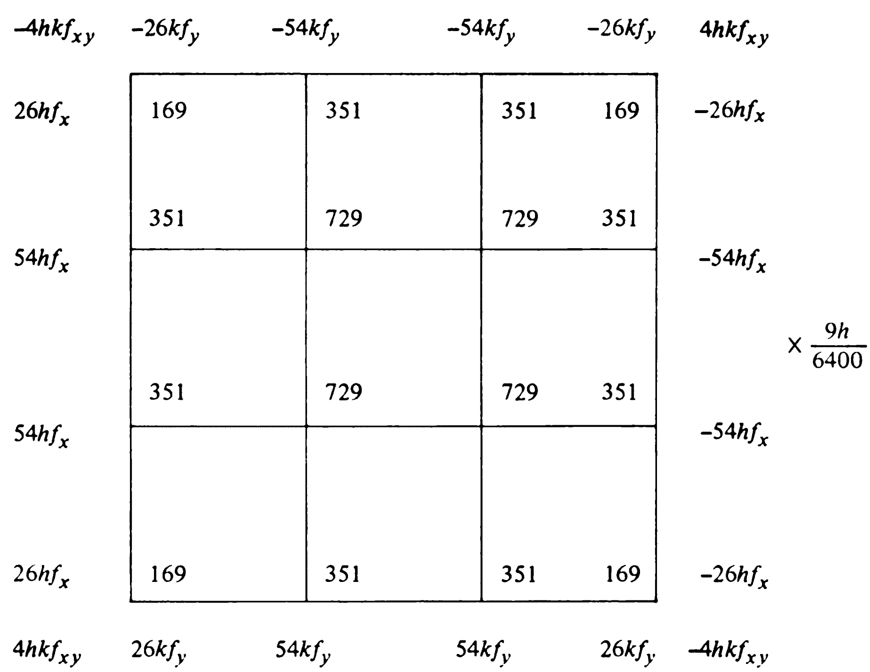


Figure 5.2.8 DC Simpson's Second Rule

5^2 Point Rule

$$A^{(1,1)(4,1)(4,4)}_{(1,0)(1,1)}(h,k) = [256\,T_{11} - 16\,T_{41} + T_{44}]/225$$

$$= I(f) - \frac{Q_{30}}{720} - \frac{E_{33}}{2025} - \frac{17E_{53}}{85\,050} - \frac{289E_{55}}{3\,572\,100} + \cdots \tag{5.2.7}$$

$$+ \, b_{2s}\Bigg[Q_{2s-1,0} + \frac{1}{225}\sum_{\beta=1}^{s} b_{2\beta}[256 - 16(16^s + 16^\beta)$$

$$+ \, 16^{s+\beta}]\,E_{2s-1,2\beta-1}\Bigg] + \Omega(h,k;2s,2s).$$

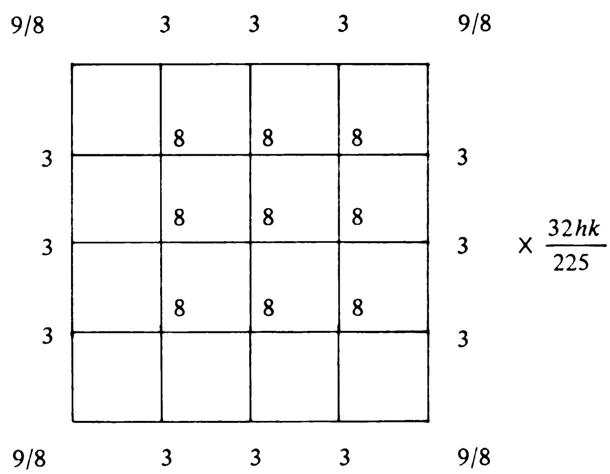


Figure 5.2.9 5^2 Point Rule

DC 5^2 Rule

$$A^{(1,1)(4,1)(4,4)}_{(3,0)(3,1)}(h,k) = [65\,536\,T_{11} - 256\,T_{41} + T_{44}]/65\,025 - \frac{Q_{10}}{12} + \frac{16E_{11}}{2601}$$

$$= I(f) + \frac{Q_{50}}{30\,240} - \frac{32E_{51}}{819\,315} - \frac{64E_{55}}{258\,084\,225} + \cdots \qquad (5.2.8)$$

$$+ b_{2s}\left[Q_{2s-1,0} + \frac{1}{65\,025}\sum_{\beta=1}^{s} b_{2\beta}[65\,536 - 256\,(16^s + 16^\beta)\right.$$

$$\left. + 16^{s+\beta}]\,E_{2s-1,2\beta-1}\right] + \Omega(h,k;2s,2s).$$

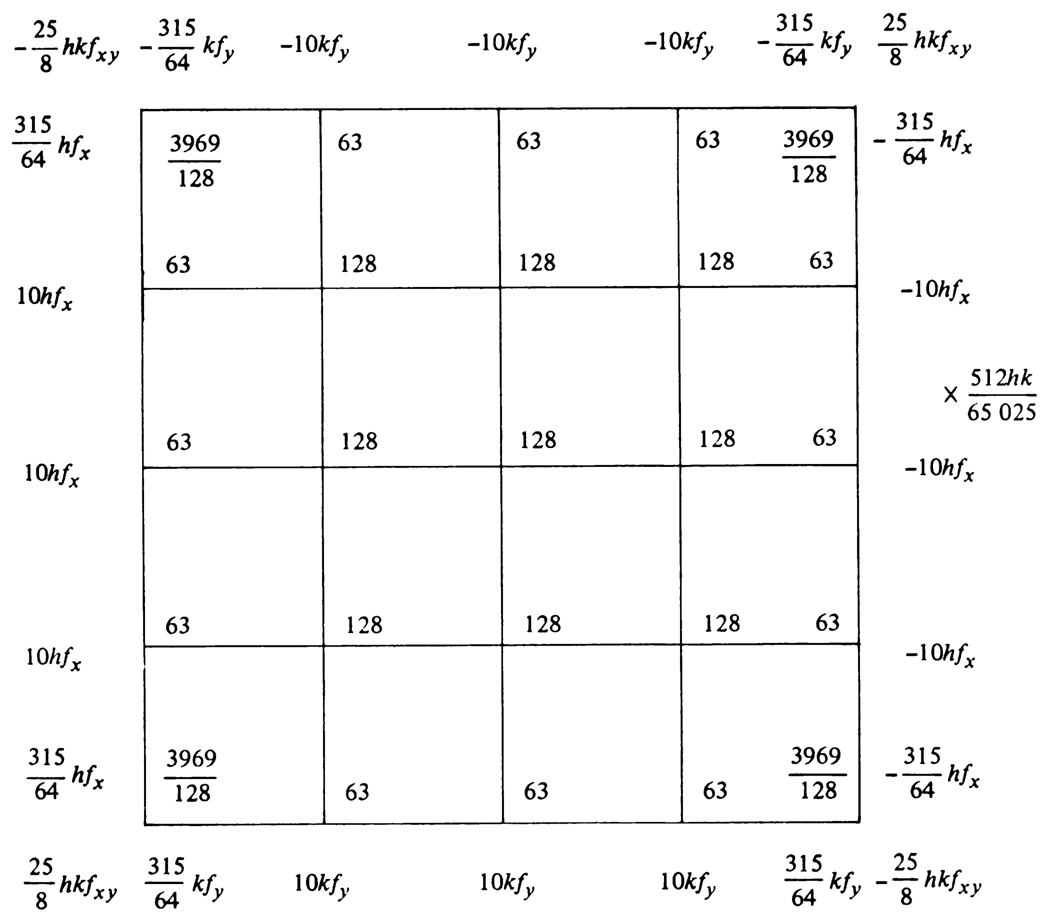


Figure 5.2.10 DC 5^2 Rule

Boole's Rule

$$
\begin{aligned}
B(h,k) &= A^{(1,1)(2,1)(2,2)(4,1)(4,2)(4,4)}_{(1,0)(1,1)(3,0)(3,1)(3,3)}(h,k) \\
&= [4096\,T_{11} - 1280\,T_{21} + 400\,T_{22} + 64\,T_{41} - 20\,T_{42} + T_{44}]/2025 \\
&= [256\,S_{11} - 16\,S_{12} + S_{22}]/225 \\
&= I(f) + \frac{Q_{50}}{30\,240} - \frac{4E_{55}}{893\,025} - \frac{Q_{70}}{1\,209\,600} - \frac{E_{75}}{425\,250} - \frac{E_{77}}{810\,000} + \cdots \\
&\quad + b_{2s}\Big[Q_{2s-1,0} + \frac{1}{2025}\sum_{\beta=1}^{s} b_{2\beta}[4096 - 1280(4^s + 4^\beta) + 400(4^{s+\beta}) \\
&\quad + 64(16^s + 16^\beta) - 20(4^{2s+\beta} + 4^{s+2\beta}) + 16^{s+\beta}]\,E_{2s-1,2\beta-1}\Big] + \Omega(h,k;2s,2s).
\end{aligned}
\tag{5.2.9}
$$

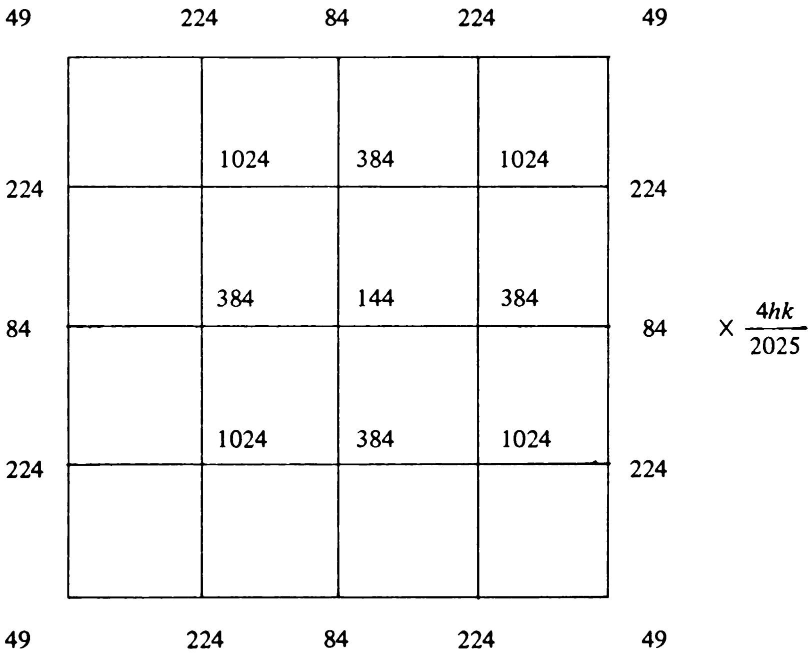


Figure 5.2.11 Boole's Rule

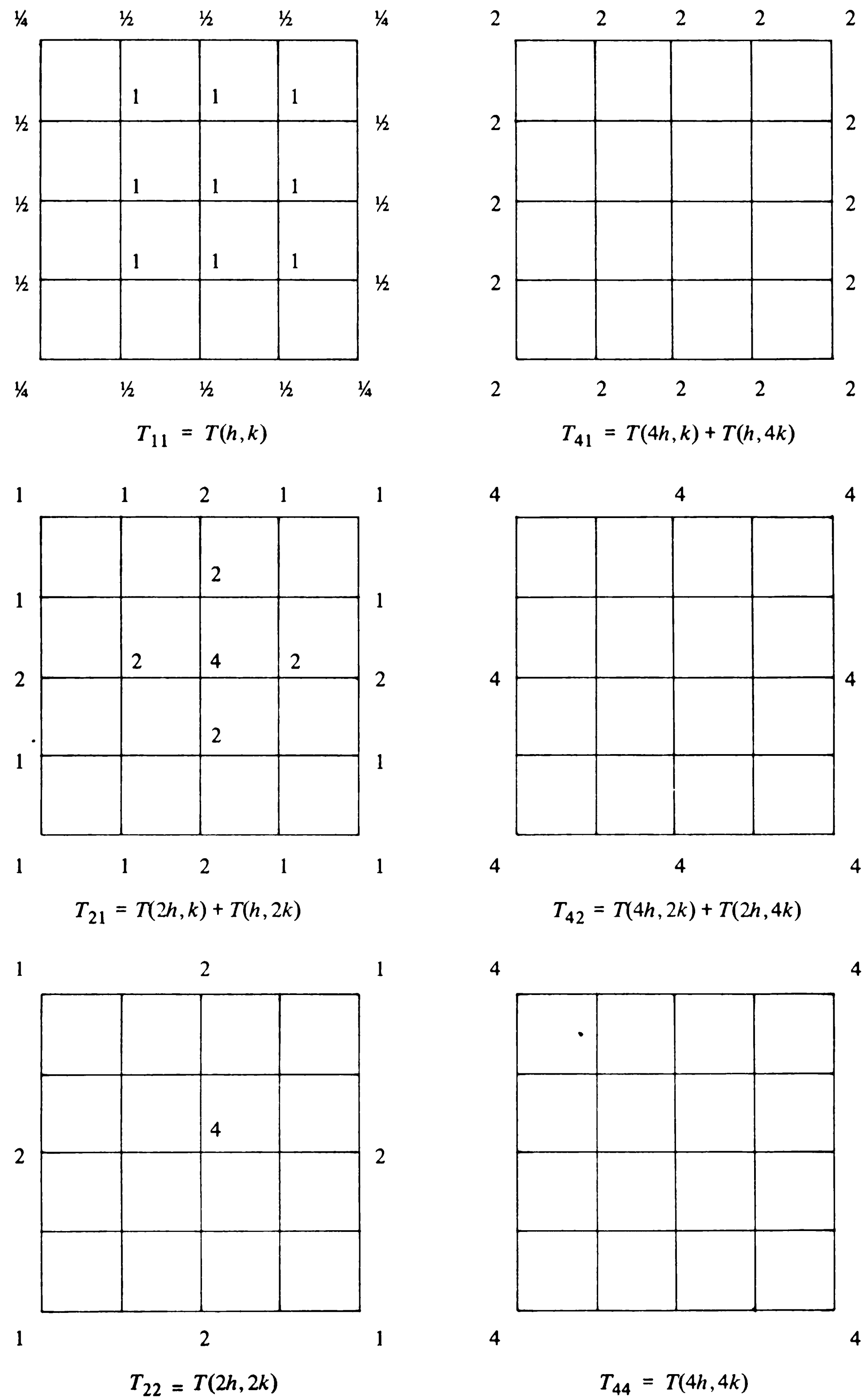


Figure 5.2.12 Component Trapezoidal Sums for Boole's Rule

DC Boole's Rule

$$B'(h,k) = A^{(1,1)(2,1)(2,2)(4,1)(4,2)(4,4)}_{(3,0)(3,1)(5,0)(3,3)(5,1)}(h,k)$$

$$= [1048\,576\,T_{11} - 81\,920\,T_{21} + 6400\,T_{22} + 1024\,T_{41} - 80\,T_{42}$$

$$+ T_{44}]/893\,025 - \frac{Q_{10}}{12} + \frac{16E_{11}}{3969}$$

$$= [4096\,s'_{11} - 64\,s'_{21} + s'_{22}]/3969$$

$$= I(f) - \frac{Q_{70}}{1\,209\,600} - \frac{16E_{71}}{6\,251\,175} - \frac{16E_{77}}{9\,845\,600\,625} + \cdots \qquad (5.2.10)$$

$$+ b_{2s}\Bigg[Q_{2s-1,0} + \frac{1}{893\,025}\sum_{\beta=1}^{s} b_{2\beta}[1\,048\,576$$

$$- 81\,920(4^s + 4^\beta) + 6400(4^{s+\beta}) + 1024(16^s + 16^\beta)$$

$$- 80(4^{2s+\beta} + 4^{s+2\beta}) + 16^{s+\beta}]\,E_{2s-1,2\beta-1}\Bigg] + \Omega(h,k;2s,2s) \qquad s = 4,5,\cdots$$

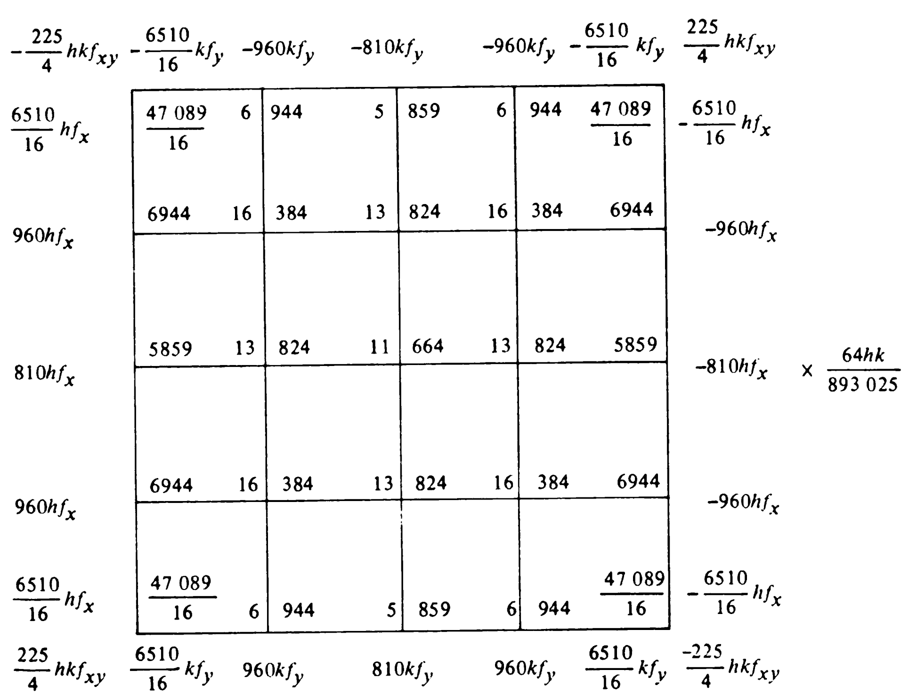


Figure 5.2.13 DC Boole's Rule

Weddle's Rule

$$A^{(1,1)(2,1)(2,2)(3,1)(3,2)(3,3)}_{(1,0)(1,1)(3,0)(3,1)(3,3)}(h,k)$$

$$= [225\,T_{11} - 90\,T_{21} + 36\,T_{22} + 15\,T_{31} - 6\,T_{32} + T_{33}]/100$$

$$= I(f) + \frac{Q_{50}}{30\,240} - \frac{Q_{70}}{1\,209\,600} - \frac{E_{75}}{2\,016\,000} - \frac{E_{77}}{5\,760\,000} + \cdots \tag{5.2.11}$$

$$+ b_{2s}\Bigg[Q_{2s-1,0} + \frac{1}{100}\sum_{\beta=1}^{s} b_{2\beta}\,[225 - 90(4^s + 4^\beta) + 36(4^{s+\beta}) + 15(9^s + 9^\beta)$$

$$- 6(9^s 4^\beta + 4^s 9^\beta) + 9^{s+\beta}]\,E_{2s-1,2\beta-1}\Bigg] + \Omega(h,k;2s,2s).$$

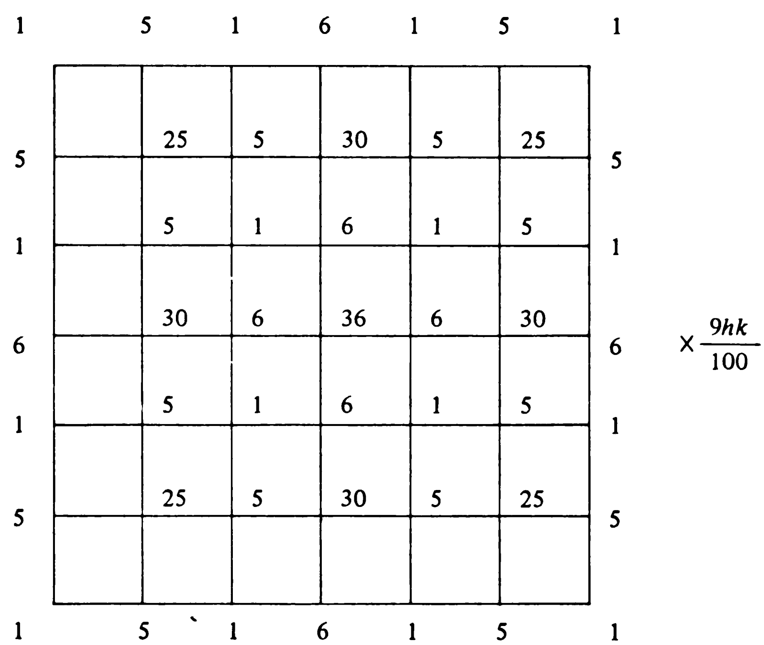


Figure 5.2.14 Weddle's Rule

DC Weddle's Rule

$$A^{(1,1)(2,1)(2,2)(3,1)(3,2)(3,3)}_{(3,0)(3,1)(3,3)(5,0)(5,1)}(h,k)$$

$$= [72\,900\,T_{11} - 7290\,T_{21} + 729\,T_{22} + 540\,T_{31} - 54\,T_{32} + 4\,T_{33}]/60\,025 - \frac{Q_{10}}{12} + \frac{9E_{11}}{2401}$$

$$= I(f) - \frac{Q_{70}}{1\,209\,600} - \frac{45E_{71}}{6\,722\,800} - \frac{9E_{77}}{18\,823\,840\,000} + \cdots \qquad (5.2.12)$$

$$+ b_{2s}\Bigg[Q_{2s-1,0} + \frac{1}{60\,025}\sum_{\beta=1}^{s} b_{2\beta}\,[72\,900 - 7290(4^s + 4^\beta) + 729(4^{s+\beta}) + 540(9^s + 9^\beta)$$

$$- 54(9^s 4^\beta + 4^s 9^\beta) + 9^{s+\beta}]\,E_{2s-1,2\beta-1}\Bigg] + \Omega(h,k;2s,2s).$$

$-25hkf_{xy}$	$-185kf_y$		$-450kf_y$		$-360kf_y$		$-460kf_y$		$-360kf_y$		$-450kf_y$	$-185kf_y$	$25hkf_{xy}$
$185hf_x$	1369	3	330	2	664	3	404	2	664	3	330	1369	$-185hf_x$
$450hf_x$	3330	8	100	6	480	8	280	6	480	8	100	3330	$-450hf_x$
$360hf_x$	2664	6	480	5	184	6	624	5	184	6	480	2664	$-360hf_x$
$460hf_x$	3404	8	280	6	624	8	464	6	624	8	280	3404	$-460hf_x$
$360hf_x$	2664	6	480	5	184	6	624	5	184	6	480	2664	$-360hf_x$
$450hf_x$	3330	8	100	6	480	8	280	6	480	8	100	3330	$-450hf_x$
$185hf_x$	1369	3	330	2	664	3	404	2	664	3	330	1369	$-185hf_x$
$25hkf_{xy}$	$185kf_y$		$450kf_y$		$360kf_y$		$460kf_y$		$360kf_y$		$450kf_y$	$185kf_y$	$-25hkf_{xy}$

$$\times \frac{9hk}{60\,025}$$

Figure 5.2.15 DC Weddle's Rule

Newton-Cotes' 7^2 Rule

$$N(h,k) = A^{(1,1)(2,1)(2,2)(3,1)(3,2)(3,3)(6,1)(6,2)(6,3)(6,6)}_{(1,0)(1,1)(3,0)(3,1)(3,3)(5,0)(5,1)(5,3)(5,5)}(h,k)$$

$$= [1\,679\,616\,T_{11} - 734\,832\,T_{21} + 321\,489\,T_{22} + 145\,152\,T_{31} - 63\,504\,T_{32} + 12\,544\,T_{33}$$

$$- 1296\,T_{61} + 567\,T_{62} - 112\,T_{63} + T_{66}]/705\,600$$

$$= I(f) - \frac{Q_{70}}{1\,209\,600} - \frac{9E_{77}}{7\,840\,000} + \frac{Q_{90}}{47\,900\,160} - \frac{E_{97}}{689\,920} - \frac{25E_{99}}{13\,660\,416} + \cdots \tag{5.2.13}$$

$$+ b_{2s}\Bigg[Q_{2s-1,0} + \frac{1}{705\,600}\sum_{\beta=1}^{s} b_{2\beta}[1\,679\,616 - 734\,832(4^s + 4^\beta) + 321(4^{s+\beta})$$

$$+ 145\,152(9^s + 9^\beta) - 63\,504(9^s 4^\beta + 4^s 9^\beta) + 12\,544(9^{s+\beta}) - 1296(36^s + 36^\beta)$$

$$+ 567(36^s 4^\beta + 4^s 36^\beta) - 112(36^s 9^\beta + 9^s 36^\beta) + 36^{s+\beta}]E_{2s-1,2\beta-1}\Bigg] + \Omega(h,k;2s,2s).$$

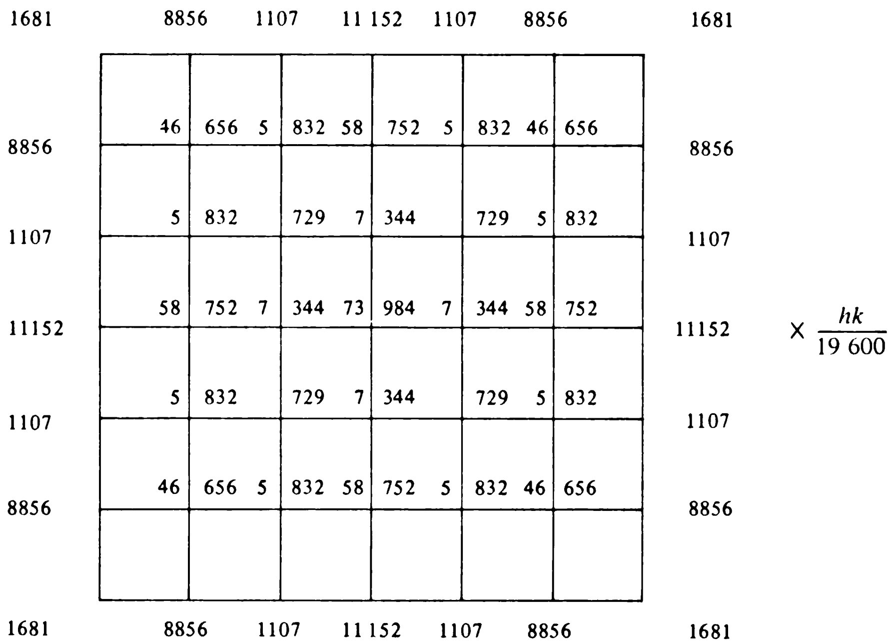
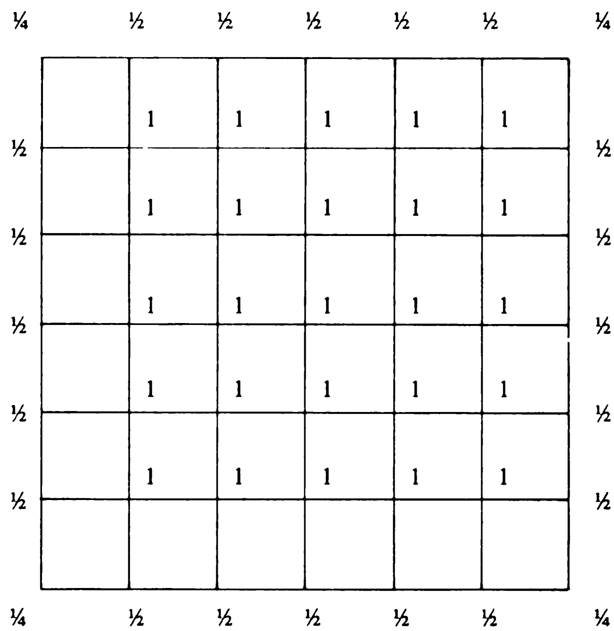
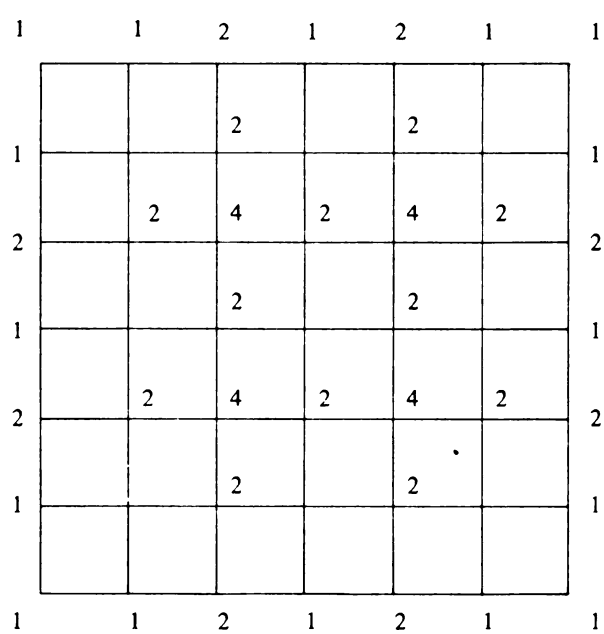


Figure 5.2.16 Newton-Cotes' 7^2 Rule

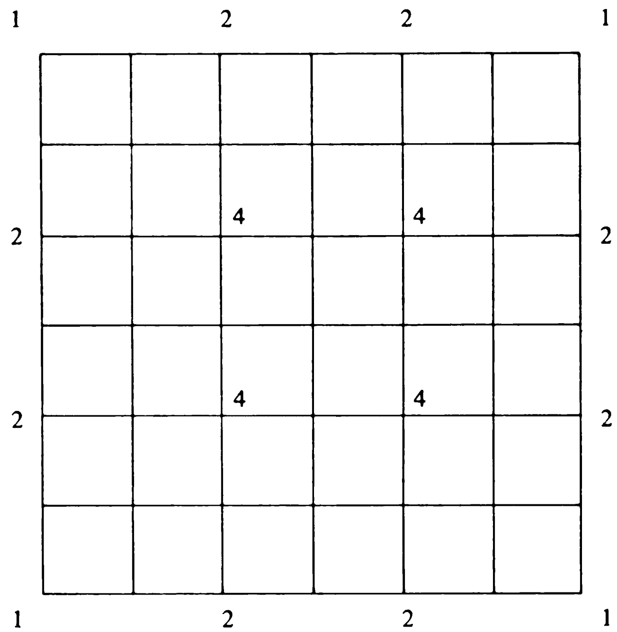


$T_{11} = T(h,k)$

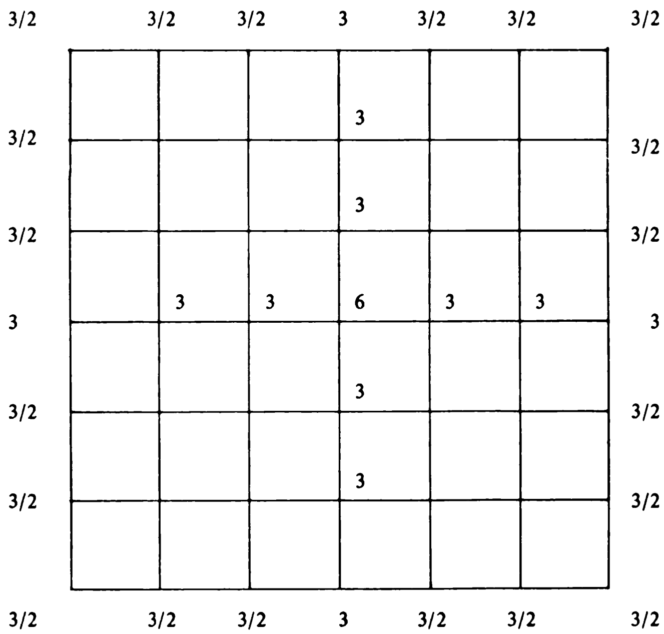


$T_{21} = T(2h,k) + T(h,2k)$

Figure 5.2.17 Component Trapezoidal Sums for Newton-Cotes' 7^2 Rule

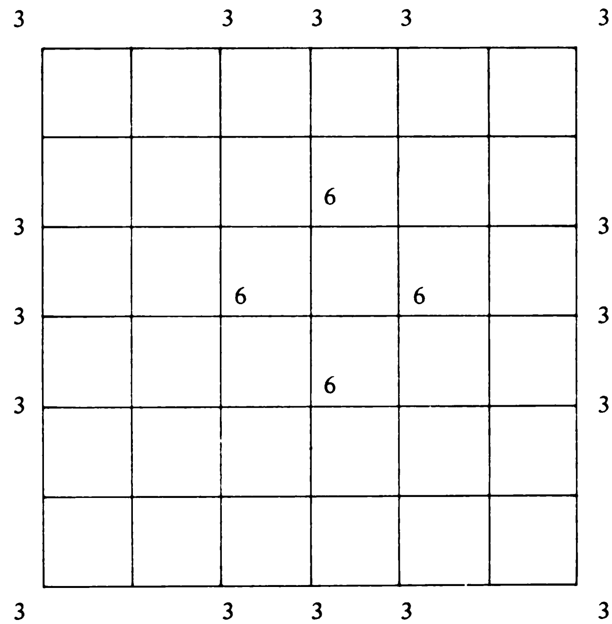


$T_{22} = T(2h, 2k)$

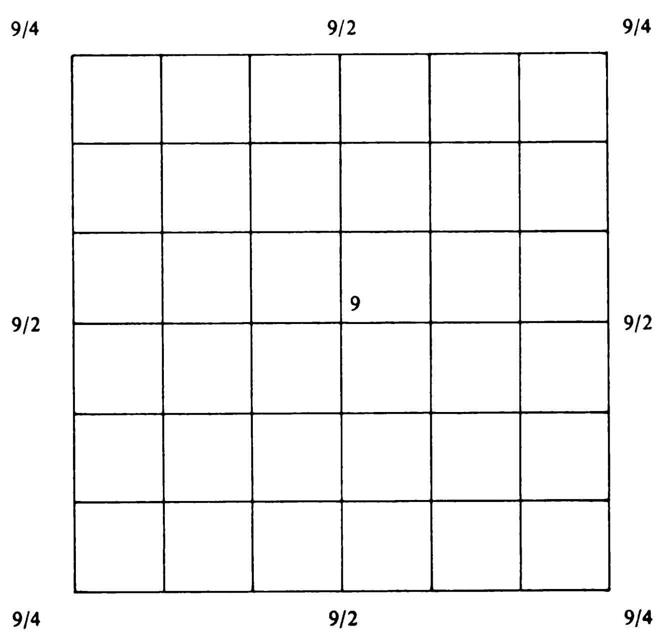


$T_{31} = T(3h, k) + T(h, 3k)$

Figure 5.2.17 (cont'd.)

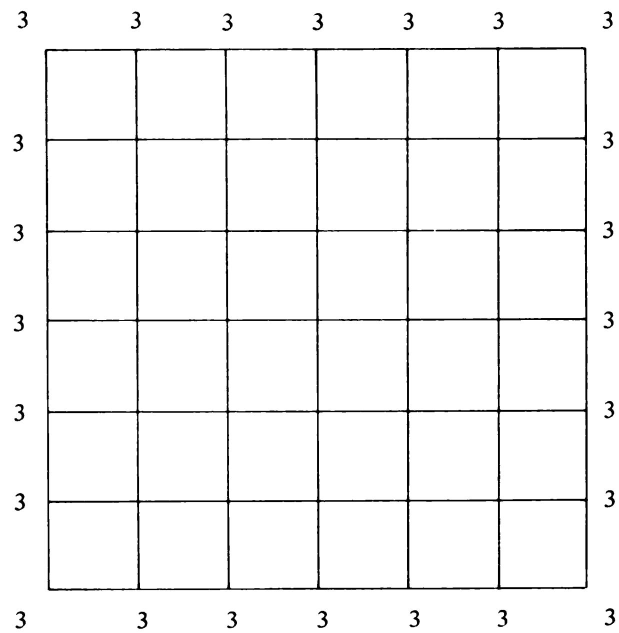


$T_{32} = T(3h, 2k) + T(2h, 3k)$

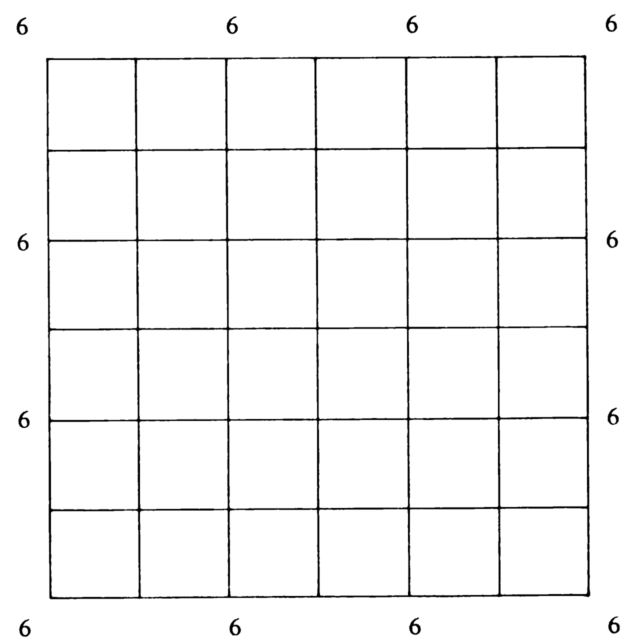


$T_{33} = T(3h, 3k)$

Figure 5.2.17 (cont'd.)

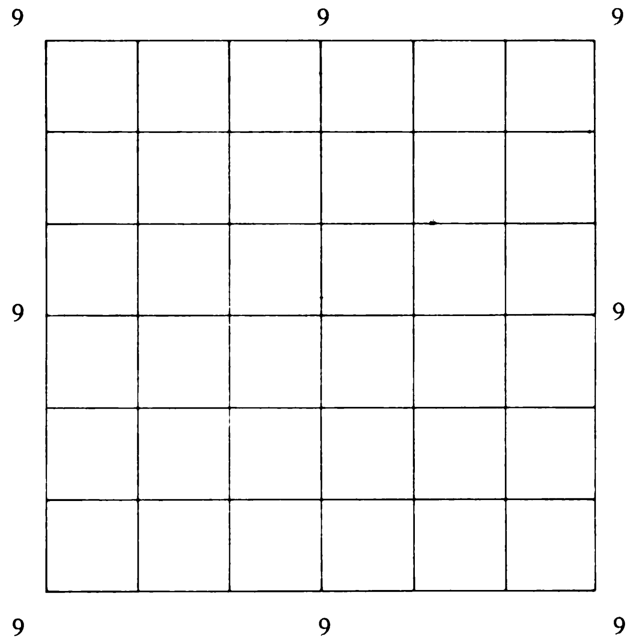


$T_{61} = T(6h, k) + T(h, 6k)$

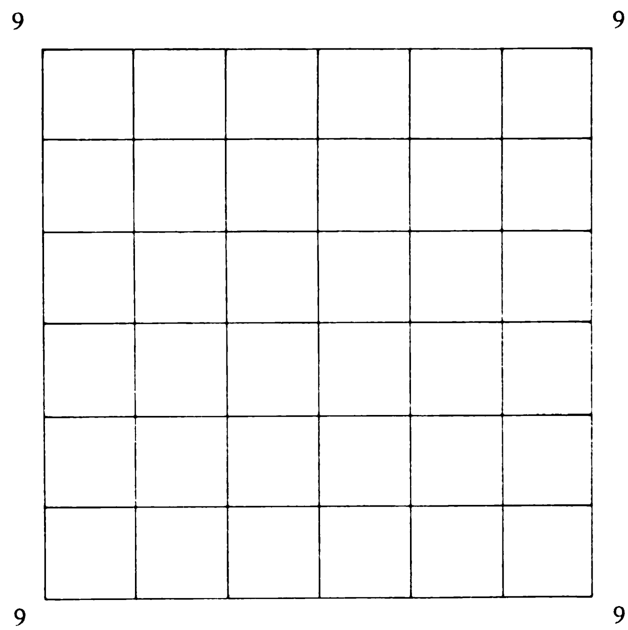


$T_{62} = T(6h, 2k) + T(2h, 6k)$

Figure 5.2.17 (cont'd.)



$T_{63} = T(6h, 3k) + T(3h, 6k)$



$T_{66} = T(6h, 6k)$

Figure 5.2.17 (cont'd.)

DC Newton-Cotes' 7^2 Rule

$$N'(h,k) = A^{(1,1)(2,1)(2,2)(3,1)(3,2)(3,3)(6,1)(6,2)(6,3)(6,6)}_{(3,0)(3,1)(3,3)(5,0)(5,1)(5,3)(5,5)(7,0)(7,3)}(h,k)$$

$$= [2\,176\,782\,336\,T_{11} - 238\,085\,568\,T_{21}$$

$$+ 26\,040\,609\,T_{22} + 20\,901\,888\,T_{31} - 2\,286\,144\,T_{32} + 200\,704\,T_{33}$$

$$- 46\,656\,T_{61} + 5103\,T_{62} - 448\,T_{63} + T_{66}]/1\,764\,000\,000$$

$$- \frac{Q_{10}}{12} + \frac{9E_{11}}{2500}$$

$$= I(f) + \frac{Q_{90}}{47\,900\,160} - \frac{9E_{91}}{7\,700\,000} - \frac{9E_{99}}{23\,716\,000\,000} + \cdots \qquad (5.2.14)$$

$$+ b_{2s}\Bigg[Q_{2s-1,0} + \frac{1}{1\,764\,000\,000}\sum_{\beta=1}^{s} b_{2\beta}[2\,176\,782\,336 - 238\,085\,568(4^s + 4^\beta)$$

$$+ 26\,040\,609(4^{s+\beta}) + 20\,901\,888(9^s + 9^\beta) - 2\,286\,144(9^s4^\beta + 4^s9^\beta)$$

$$+ 200\,704(9^{s+\beta}) - 46\,656(36^s + 36^\beta) + 5103(36^s4^\beta + 4^s36^\beta)$$

$$- 448(36^s9^\beta + 9^s36^\beta) + 36^{s+\beta}]\,E_{2s-1,2\beta-1}\Bigg]$$

$$+ \Omega(h,k;2s,2s).$$

$-17\,6400hkf_{xy}$	$-132\,2580kf_y$	$-326\,5920kf_y$	$-255\,1500kf_y$	$-336\,0000kf_y$	$-255\,1500kf_y$	$-326\,5920kf_y$	$-132\,2580kf_y$	$17\,6400hkf_{xy}$
$132\,2580hf_x$	991 6201	2448 6624	1913 0175	2519 2000	1913 0175	2448 6624	991 6201	$-132\,2580hf_x$
$326\,5920hf_x$	2448 6624	6046 6176	4723 9200	6220 8000	4723 9200	6046 6176	2448 6624	$-326\,5920hf_x$
$255\,1500hf_x$	1913 0175	4723 9200	3690 5625	4860 0000	3690 5625	4723 9200	1913 0175	$-255\,1500hf_x$
$336\,0000hf_x$	2519 2000	6220 8000	4860 0000	6400 0000	4860 0000	6220 8000	2519 2000	$-336\,0000hf_x$
$255\,1500hf_x$	1913 0175	4723 9200	3690 5625	4860 0000	3690 5625	4723 9200	1913 0175	$-255\,1500hf_x$
$326\,5920hf_x$	2448 6624	6046 6176	4723 9200	6220 8000	4723 9200	6046 6176	2448 6624	$-326\,5920hf_x$
$132\,2580hf_x$	991 6201	2448 6624	1913 0175	2519 2000	1913 0175	2448 6624	991 6201	$-132\,2580hf_x$
$17\,6400hkf_{xy}$	$132\,2580kf_y$	$326\,5920kf_y$	$255\,1500kf_y$	$336\,0000kf_y$	$255\,1500kf_y$	$326\,5920kf_y$	$132\,2580kf_y$	$-17\,6400hkf_{xy}$

$$\times \frac{hk}{49\,000\,000}$$

Figure 5.2.18 DC Newton-Cotes' 7^2 Rule

Romberg's 9^2-Point Rule

$$A^{(1,1)(2,1)(2,2)(4,1)(4,2)(4,4)(8,1)(8,2)(8,4)(8,8)}_{(1,0)(1,1)(3,0)(3,1)(3,3)(5,0)(5,1)(5,3)(5,5)}(h,k)$$

$$= [16\,777\,216\,T_{11} - 5\,505\,024\,T_{21} + 1\,806\,336\,T_{22}$$

$$+ 344\,064\,T_{41} - 112\,896\,T_{42} + 7\,056\,T_{44}$$

$$- 4\,096\,T_{81} + 1\,344\,T_{82} - 84\,T_{84} + T_{88}]/8\,037\,225$$

$$= [4\,096\,B_{11} - 64\,B_{21} + B_{22}]/3969$$

$$= I(f) - \frac{Q_{70}}{1\,209\,600} - \frac{256E_{77}}{22\,325\,625} + \frac{Q_{90}}{47\,900\,160} - \frac{2176E_{97}}{88\,409\,475} - \frac{18\,496E_{99}}{350\,101\,521} + \cdots \tag{5.2.15}$$

$$+ b_{2s}\Bigg[Q_{2s-1,0} + \frac{1}{8\,037\,225}\sum_{\beta=1}^{s} b_{2\beta}[16\,777\,216 - 5505(4^s + 4^\beta)$$

$$+ 1806\,336(4^{s+\beta}) + 344\,064(16^s + 16^\beta) - 112\,896(16^s4^\beta + 4^s16^\beta)$$

$$+ 7056(16^{s+\beta}) - 4096(64^s + 64^\beta) + 1344(64^s4^\beta + 4^s64^\beta)$$

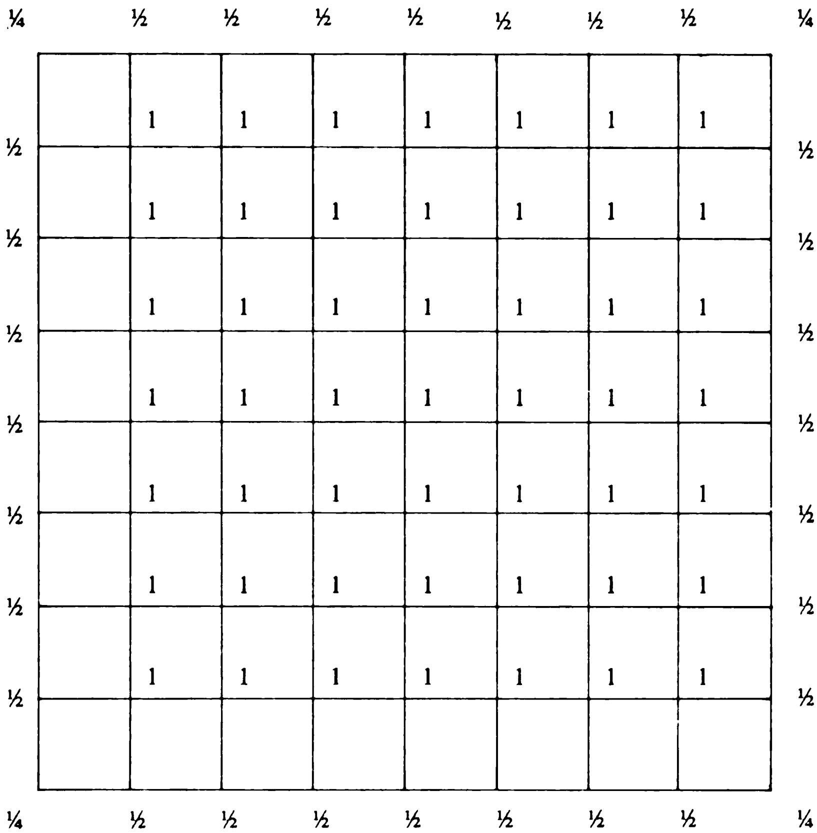
$$- 84(64^s16^\beta + 16^s64^\beta) + 64^{s+\beta}]E_{2s-1,2\beta-1}\Bigg]$$

$$+ \Omega(h,k;2s,2s).$$

4 7089	22 2208	7 6384	22 2208	9 4612	22 2208	7 6384	22 2208	4 7089
22 2208	104 8576	36 0448	104 8576	44 6464	104 8576	36 0448	104 8576	22 2208
7 6384	36 0448	12 3904	36 0448	15 3472	36 0448	12 3904	36 0448	7 6384
22 2208	104 8576	36 0448	104 8576	44 6464	104 8576	36 0448	104 8576	22 2208
9 4612	44 6464	15 3472	44 6464	19 0096	44 6464	15 3472	44 6464	9 4612
22 2208	104 8576	36 0448	104 8576	44 6464	104 8576	36 0448	104 8576	22 2208
7 6384	36 0448	12 3904	36 0448	15 3472	36 0448	12 3904	36 0448	7 6384
22 2208	104 8576	36 0448	104 8576	44 6464	104 8576	36 0448	104 8576	22 2208
4 7089	22 2208	7 6384	22 2208	9 4612	22 2208	7 6384	22 2208	4 7089

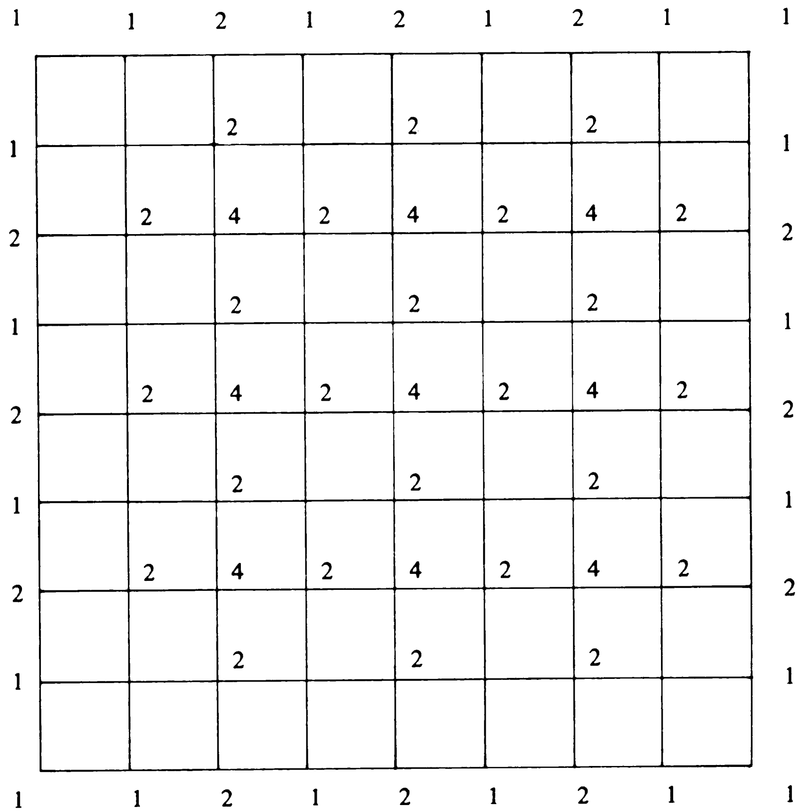
$$\times \frac{16hk}{8\,037\,226}$$

Figure 5.2.19 Romberg's 9^2-Point Rule



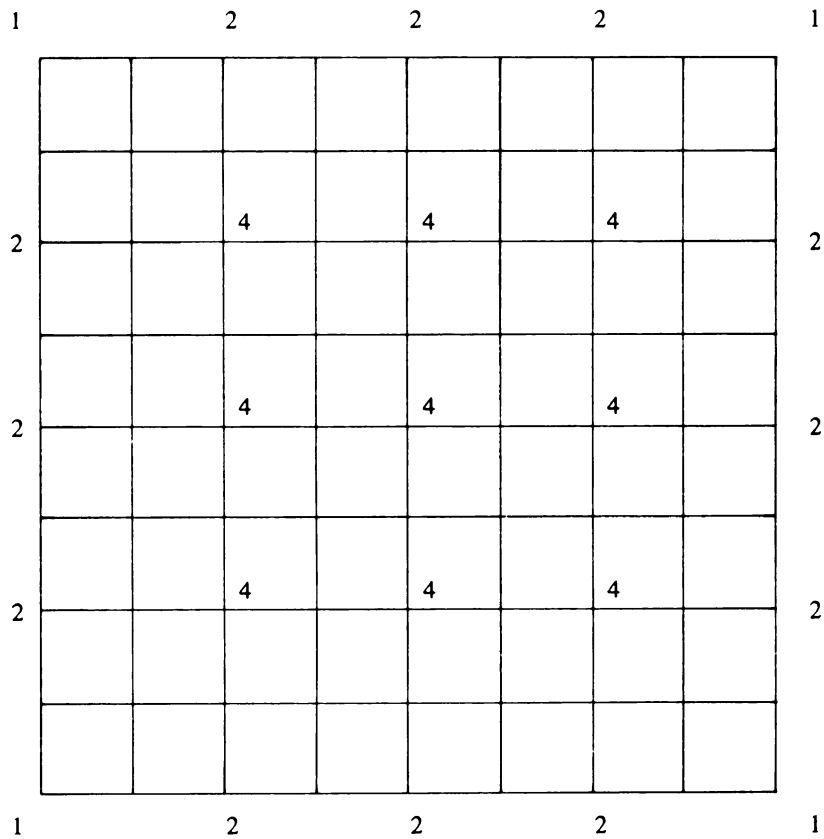
$$T_{11} = T(h,k)$$

Figure 5.2.20 Component Trapezoidal Sums for Romberg's 9^2 Rule



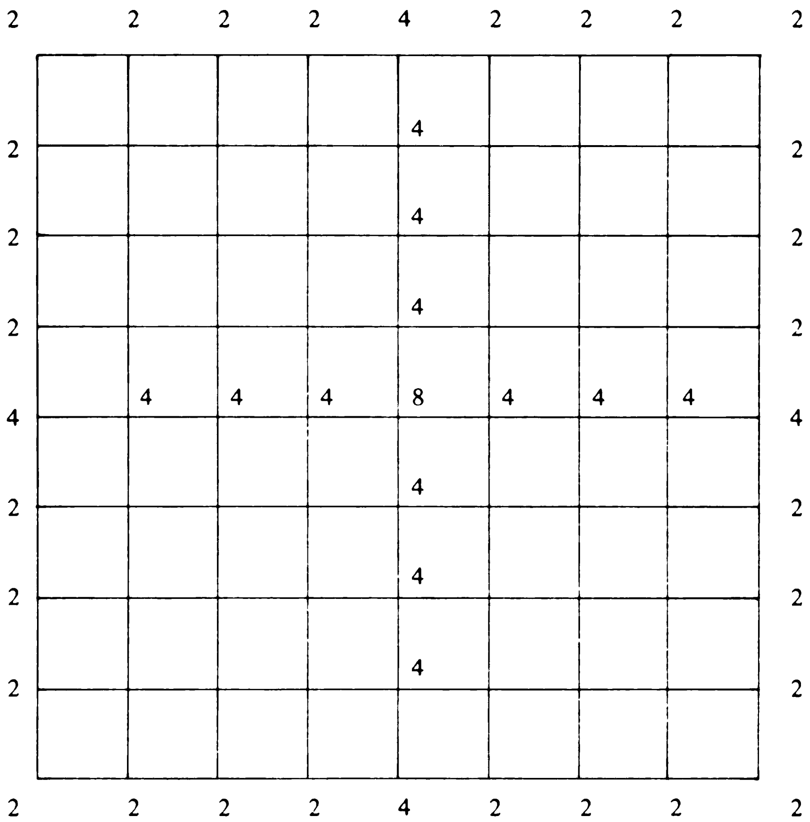
$$T_{21} = T(2h, k) + T(h, 2k)$$

Figure 5.2.20 (cont'd.)



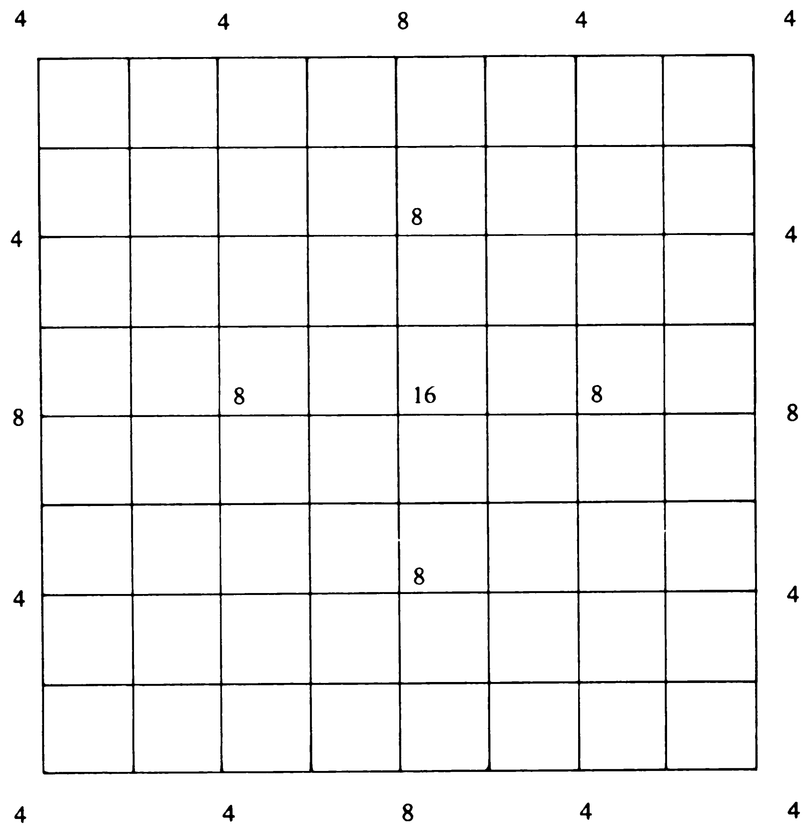
$T_{22} = T(2h, 2k)$

Figure 5.2.20 (cont'd.)



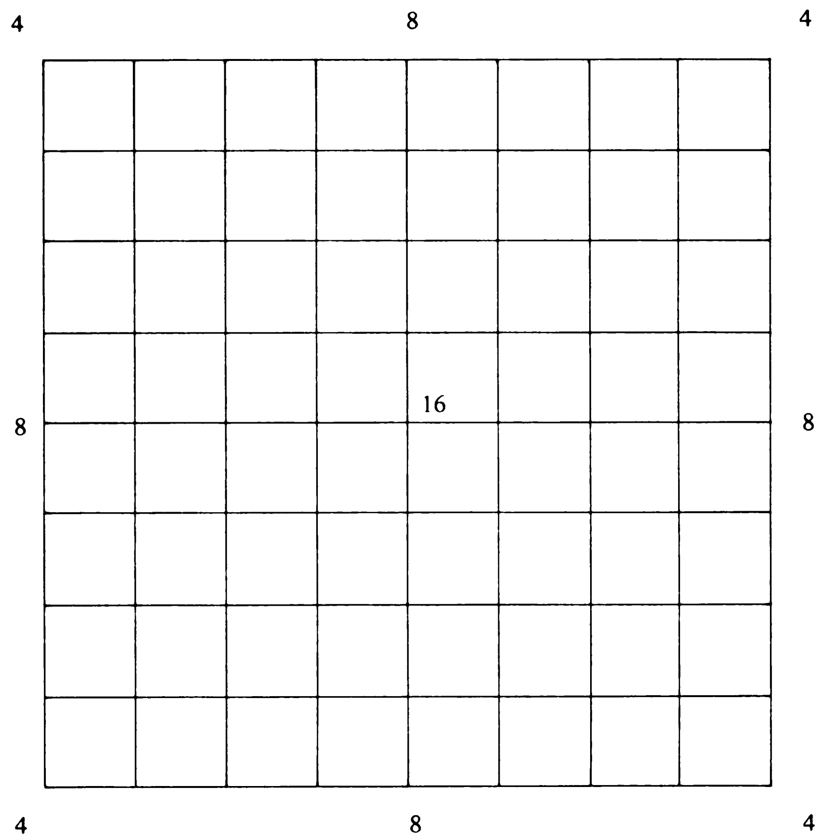
$$T_{41} = T(4h, k) + T(h, 4k)$$

Figure 5.2.20 (cont'd.)



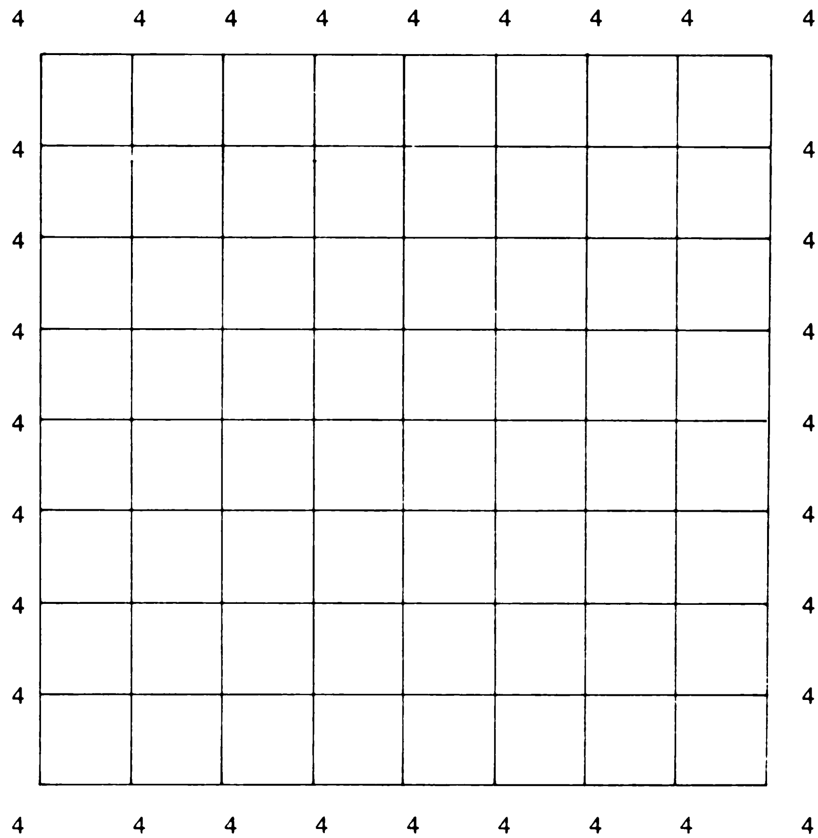
$$T_{42} = T(4h, 2k) + T(2h, 4k)$$

Figure 5.2.20 (cont'd.)



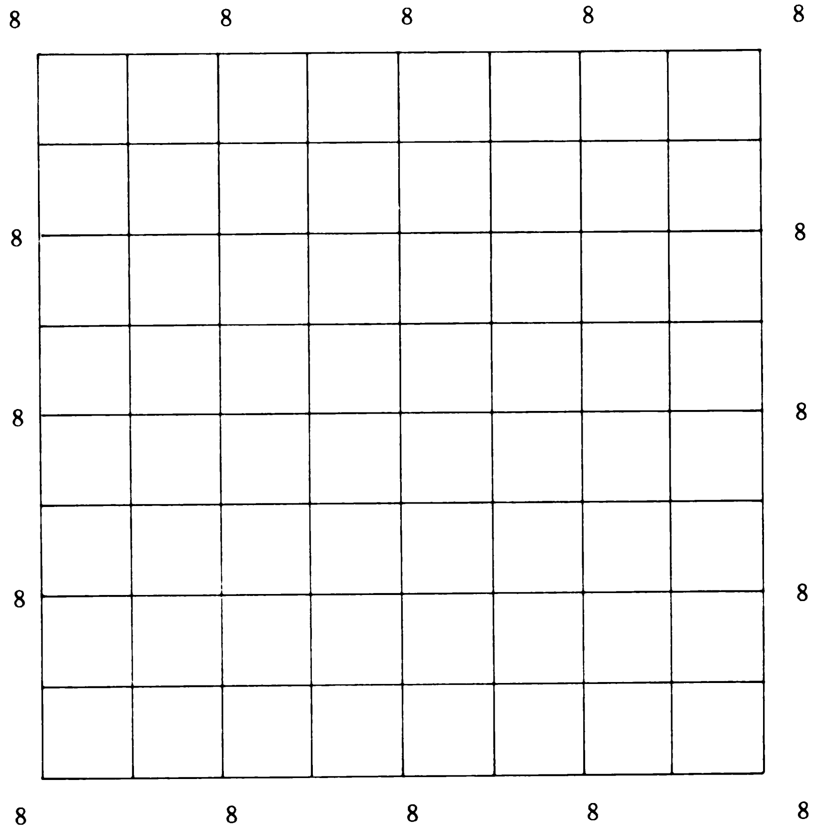
$T_{44} = T(4h, 4k)$

Figure 5.2.20 (cont'd.)



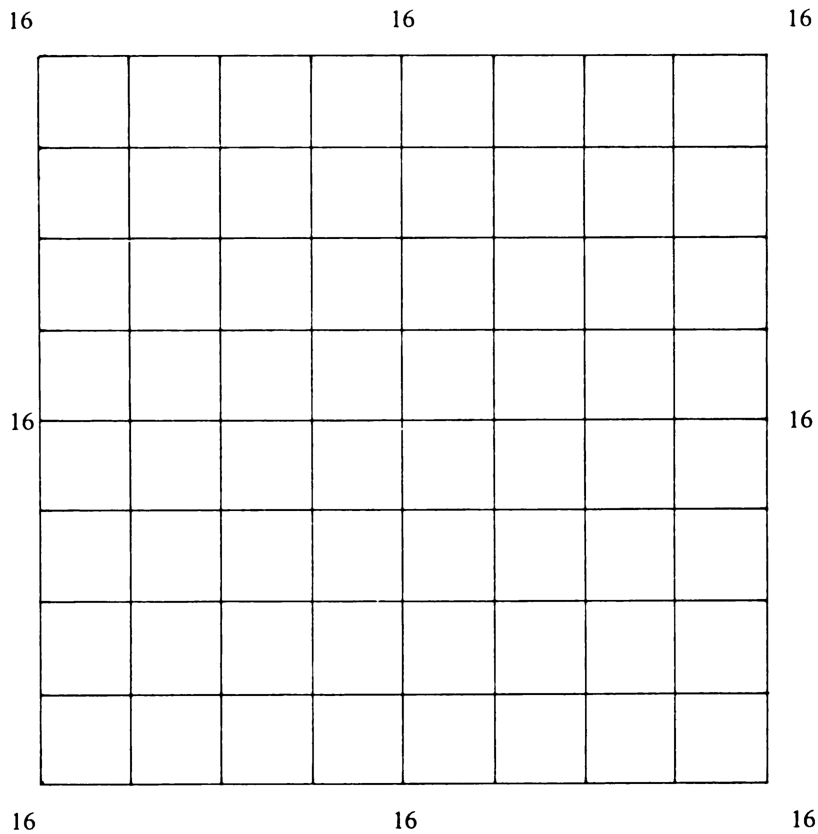
$$T_{81} = T(8h,k) + T(h,8k)$$

Figure 5.2.20 (cont'd.)



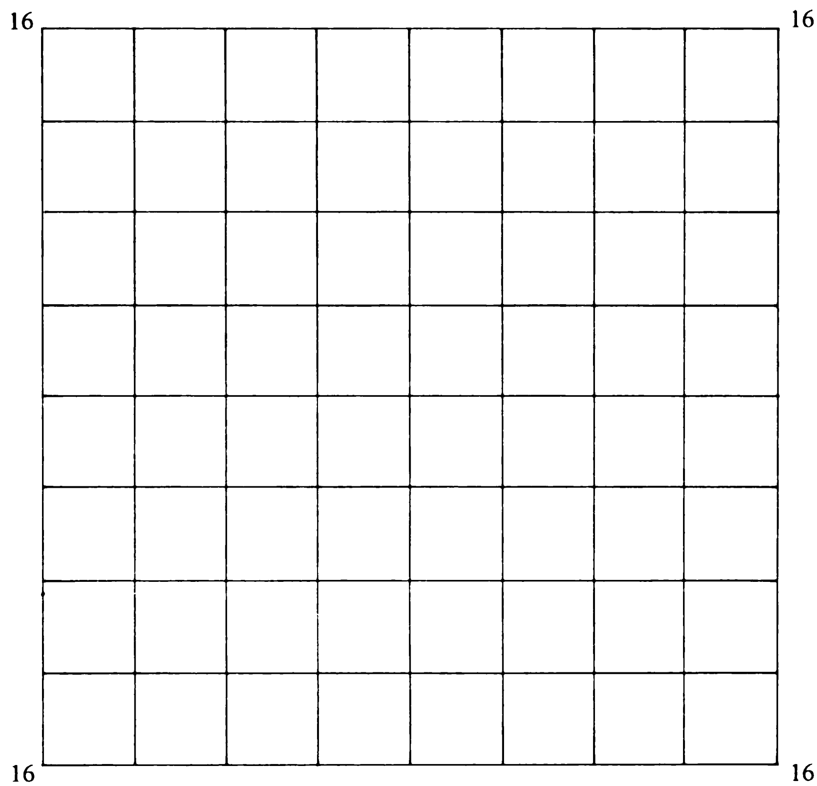
$$T_{82} = T(8h, 2k) + T(2h, 8k)$$

Figure 5.2.20 (cont'd.)



$T_{84} = T(8h, 4k) + T(4h, 8k)$

Figure 5.2.20 (cont'd.)



$T_{88} = T(8h, 8k)$

Figure 5.2.20 (cont'd.)

DC Romberg's 9^2-Point Rule

$$A^{(1,1)(2,1)(2,2)(4,1)(4,2)(4,4)(8,1)(8,2)(8,4)(8,8)}_{(3,0)(3,1)(3,3)(5,0)(5,1)(5,3)(5,5)(7,0)(7,1)}(h,k)$$

$$= [68\,719\,476\,736\,T_{11} - 5\,637\,144\,576\,T_{21} + 462\,422\,016\,T_{22}$$

$$+ 88\,080\,384\,T_{41} - 7\,225\,344\,T_{42} + 112\,896\,T_{44} - 262\,144\,T_{81}$$

$$+ 21\,504\,T_{82} - 336\,T_{84} + T_{88}]/58\,068\,950\,625 - \frac{Q_{10}}{12} + \frac{12\,544E_{11}}{3\,186\,225}$$

$$= [65\,536B'_{11} - 256B'_{21} + B'_{22}]/65\,025$$

$$= I(f) + \frac{Q_{90}}{47\,900\,160} - \frac{8\,192E_{91}}{2\,027\,804\,625} - \frac{262\,144E_{99}}{63\,237\,087\,230\,625} + \cdots$$

(5.2.16)

$$+ b_{2s}\Bigg[Q_{2s-1,0} + \frac{1}{(240\,975)^2}\sum_{\beta=1}^{s} b_{2\beta}[68\,719\,476\,736$$

$$- 5\,637\,144\,576(4^s + 4^\beta) + 462\,422\,016(4^{s+\beta})$$

$$+ 88\,080\,384(16^s + 16^\beta) - 7\,225\,344(16^s 4^\beta + 4^s 16^\beta)$$

$$+ 112\,896(16^{s+\beta}) - 262\,144(64^s + 64^\beta)$$

$$+ 21\,504(64^s 4^\beta + 4^s 64^\beta) - 336(64^s 16^\beta + 16^s 64^\beta) + 64^{s+\beta}]E_{2s-1,2\beta-1}\Bigg]$$

$$+ \Omega(h,k;2s,2s).$$

5.3 THE MIDPOINT RULE AND VARIOUS OTHER FORMULAS

The double Euler-Maclaurin Summation formula (5.2.1) may be used to derive an asymptotic expansion for the midpoint or centroid formula $C(h,k)$ by writing

$$C(h,k) = 4T\left(\frac{h}{2},\frac{k}{2}\right) - 2\left[T\left(\frac{h}{2},k\right) + T\left(h,\frac{k}{2}\right)\right] + T(h,k)$$

$$= hk\sum_{j=1}^{m}\sum_{i=1}^{n} f(a + ih/2,\ c + jk/2) \tag{5.3.1}$$

$$= \int_c^d\int_a^b f(x,y)dxdy + \cdots.$$

If the first- and mixed second-order partial derivative correction terms in (5.3.1) are transposed, a third-order derivative corrected midpoint formula analogous to (3.4.5) is obtained. The resulting DC midpoint formula is the same as formula EX183S of Table 6.4.1 and consequently the details are not given here.

The technique described in Section 5.1 may be applied to (5.3.1) to obtain a number of open cubature rules including generalizations of the open quadrature rules of Section 3.4. Because of space limitations, the results will be omitted. However, we will indicate how to obtain asymptotic expansions for several nonproduct cubature formulas.

Figures 5.3.1 to 5.3.4 illustrate Squire's [48], Ewing's [16], Tyler's [51] and Miller's [35] cubature rules.

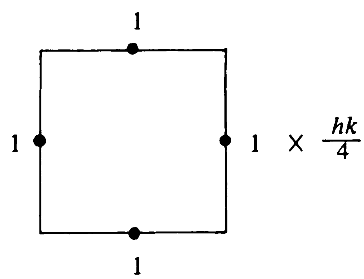


Figure 5.3.1 Squire's Rule

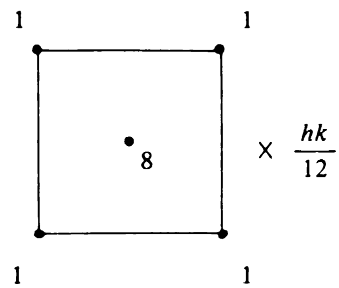


Figure 5.3.2 Ewing's Rule

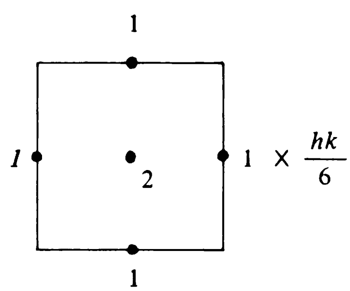


Figure 5.3.3 Tyler's Rule

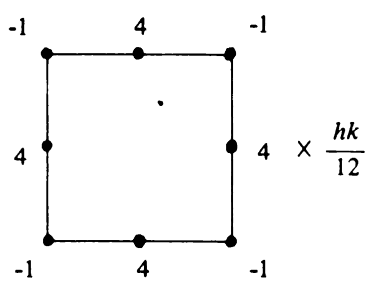


Figure 5.3.4 Miller's Rule

Asymptotic expansions for these rules may be obtained from the following:

$$\text{Squire} = -T(h,k) + [T(h,k/2) + T(h/2,k)]$$

$$\text{Ewing} = T(h,k) - \frac{4}{3}[T(h,k/2) + T(h/2,k)] + \frac{8}{3}T(h/2,k/2)$$

$$\text{Tyler} = -\frac{1}{3}T(h,k) + \frac{4}{3}T(h/2,k/2) \qquad (5.3.2)$$

$$\text{Miller} = -\frac{5}{3}T(h,k) + \frac{4}{3}[T(h,k/2) + T(h/2,k)].$$

These expansions are believed to be new. Another approach to these 4 cubature formulas is via the Taylor series; this is done in Chapter 6.

5.4 A NUMERICAL EXAMPLE

The results of applying the midpoint and DC midpoint rules to the double integral

$$\int_0^1 \int_0^1 e^{xy} dxdy \simeq 1.317\,902\,151\,454\,4 \qquad (5.4.1)$$

for grid sizes of $h = k = 1/5$ and $h = k = 1/10$ are shown in Table 5.4.1.

Table 5.4.1 Several Cubature Rules Applied to $\int_0^1 \int_0^1 e^{xy} dxdy =$ 1.317 902 151 454 4

Rule	$h = k = 1/5$		$h = k = 1/10$	
	nfe*	Error	nfe	Error
Midpoint	25	1.65-3†	100	4.16-4
DC Midpoint	49	-1.22-6	144	-7.62-8

*Number of function evaluations
†This means 1.65×10^{-3}

The DC Simpson's rule shows a similar improvement over Simpson's formula. Additional numerical results are given in Chapter 7.

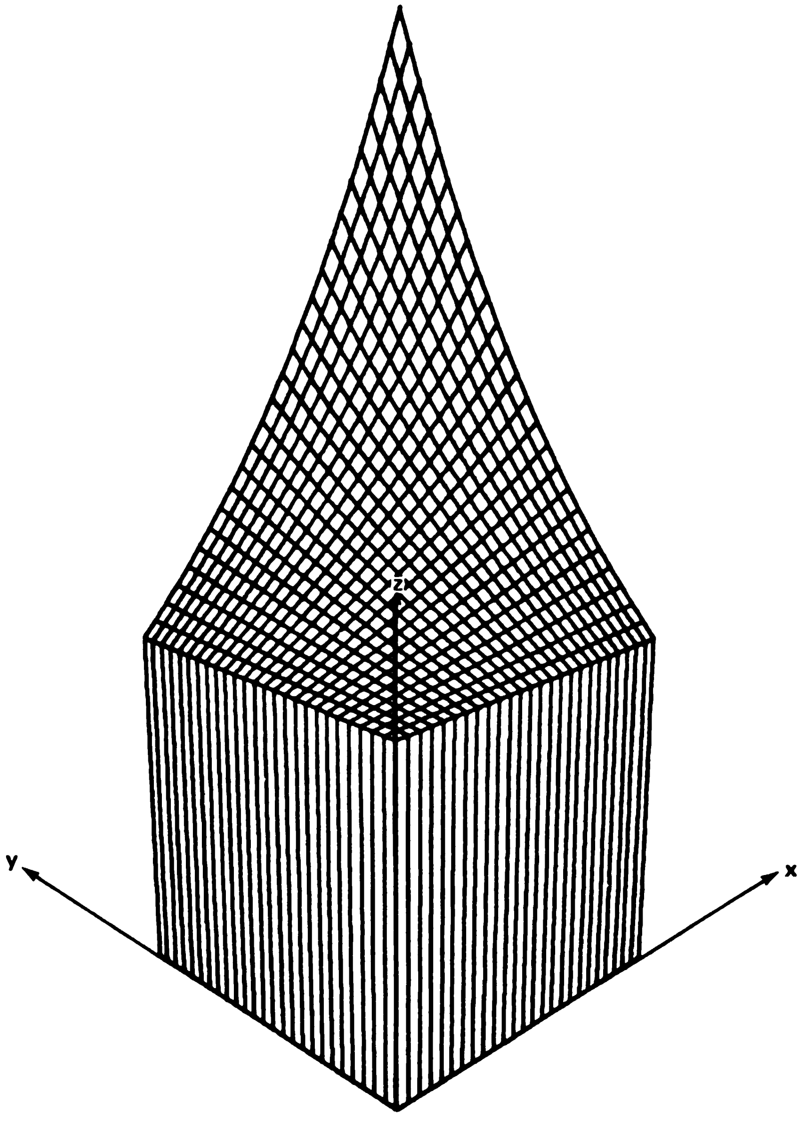


Figure 5.4.1 Graph of $z = e^{xy}$ on $[0,1]^2$

6 MULTIDIMENSIONAL QUADRATURE FORMULAS WITH PARTIAL DERIVATIVE CORRECTION TERMS

6.1 THE EQUAL WEIGHT-ALTERNATE SIGN PROPERTY

Let $f(x_1, \cdots, x_N)$ be a real valued function defined on the symmetrically placed N-dimensional rectangle

$$R = \prod_{j=1}^{N} [-h_j, h_j], \quad N \geqslant 2.$$

We wish to estimate the multiple integral

$$I(f) = \int_{-h_N}^{h_N} \cdots \int_{h_1}^{h_1} f(x_1, \cdots, x_N) dx_1 \cdots dx_N \tag{6.1.1}$$

by a multidimensional quadrature formula with partial derivative correction terms.

Partial derivatives are denoted by

$$\mathcal{D}_k^{\delta} \cdots \mathcal{D}_j^{\beta} \mathcal{D}_i^{a} f(x_1, \cdots, x_N) \tag{6.1.2}$$

where $\mathcal{D}_i^a$ denotes the a-th partial derivative of f with respect to the i-th variable.

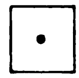
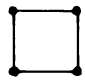
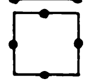
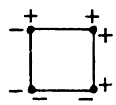
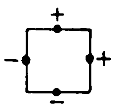
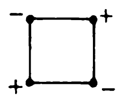
Before proceeding we make several observations for the specific case $N = 2$.

The study of the Euler-Maclaurin Summation formula for a function of two variables led to an investigation to search for additional cubature formulas involving first- and perhaps second-order partial derivative correction terms with weights of equal magnitude and alternate signs at the four corners or at the midpoints of the sides of the rectangular domain of integration so that when the rule was compounded or repeated, the weights would cancel except on the boundary. We call this the "equal-weight, alternate-sign property."

The objective is to select nodes and weights which result in efficient cubature formulas of high precision. In this connection we observe that for a composite formula of given degree of precision, a rule in which most of the nodes coincide with the boundary will be more efficient than one in which almost all of the nodes lie in the interior of the domain of integration. Moreover, additional economy can be gained by requiring the equal-weight, alternate-sign property.

Because of the endless variety of possible combinations, it was decided to limit the study to the six "cubature elements" listed in Table 6.1.1.

Table 6.1.1 Elements

Name	Cubature Element	Diagram
Centroid Value	$A_0(f) = 4h_1h_2f(0,0)$	
Corner Sum	$A_c(f) = 4h_1h_2[f(h_1,h_2)+f(-h_1,h_2)+f(-h_1,-h_2)+f(h_1,-h_2)]$	
Midpoint Sum	$A_m(f) = 4h_1h_2[f(h_1,0)+f(0,h_2)+f(-h_1,0)+f(0,-h_2)]$	
Corner, Derivative Correction	$A_c'(f) = 4h_1^2h_2[f_x(h_1,h_2)-f_x(-h_1,h_2)-f_x(-h_1,-h_2)+f_x(h_1,-h_2)]$ $+ h_1h_2^2[f_y(h_1,h_2)+f_y(-h_1,h_2)-f_y(-h_1,-h_2)-f_y(h_1,-h_2)]$	
Midpoint Derivative Correction	$A_m'(f) = 4h_1^2h_2[f_x(h_1,0)-f_x(-h_1,0)]$ $+ h_1h_2^2[f_y(0,h_2)-f_y(0,-h_2)]$	
Corner Mixed Derivative Correction	$A_c''(f) = 4h_1^2h_2^2[f_{xy}(h_1,h_2)-f_{xy}(-h_1,h_2)$ $+ f_{xy}(-h_1,-h_2)-f_{xy}(h_1,-h_2)]$	

The selection of the derivative correction cubature elements A_c', A_m', and A_c'' is based on the following considerations. For α and β nonnegative integers, define the "cubature generators" G_i listed in Table 6.1.2.

Now suppose $f(x_1,x_2)$ can be expanded in a Taylor Series about the point $(0,0)$ as far as may be required. If the series converges on R, then the G_i assume the values indicated in Table 6.1.3.

Examination of Table 6.1.3 reveals that odd/even constraints must be placed upon α and β to avoid nonzero generators G_i, which are components of the partial derivative correction elements A_c', A_m', and A_c''. These cubature elements are then candidates for inclusion in cubature formulas.

Now in order to construct multiple integration formulas with partial derivative correction terms, it is necessary to generalize the cubature elements in Table 6.1.1. Consideration of the geometry of the N-rectangle suggests how to proceed for arbitrary $N > 1$. We are now ready to derive MINTOV (an acronym for "Multiple INTegration, Order 5").

Table 6.1.2 Generators

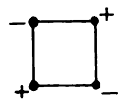
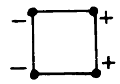
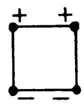
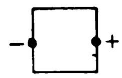
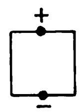
Name	Cubature Generator	Diagram
G_1	$\mathscr{S}_2^{\beta}\mathscr{S}_1^{\alpha}[f(h_1,h_2)-f(-h_1,h_2)+f(-h_1,-h_2)-f(h_1,-h_2)]$	
G_2	$\mathscr{S}_2^{\beta}\mathscr{S}_1^{\alpha}[f(h_1,h_2)-f(-h_1,h_2)-f(-h_1,-h_2)+f(h_1,-h_2)]$	
G_3	$\mathscr{S}_2^{\beta}\mathscr{S}_1^{\alpha}[f(h_1,h_2)+f(-h_1,h_2)-f(-h_1,-h_2)-f(h_1,-h_2)]$	
G_4	$\mathscr{S}_2^{\beta}\mathscr{S}_1^{\alpha}[f(h_1,0)-f(-h_1,0)]$	
G_5	$\mathscr{S}_2^{\beta}\mathscr{S}_1^{\alpha}[f(0,h_2)-f(0,-h_2)]$	

Table 6.1.3 Generator Values

α, β / Generator	α Odd β Odd	α Odd β Even	α Even β Odd	α Even β Even
G_1	Nonzero	0	0	0
G_2	0	Nonzero	0	0
G_3	0	0	Nonzero	0
G_4	0	Nonzero	0	0
G_5	0	0	Nonzero	0

6.2 DERIVATION OF MINTOV

Denote the vertices of the N-rectangle

$$R = \prod_{j=1}^{N} [-h_j, h_j]$$

by $c = (c_1, \cdots, c_N)$ where $c_j = -h_j$ or h_j, and the volume by

$$h = \prod_{j=1}^{N} 2h_j.$$

Define the sign functionals

$$\sigma_j(c) = \begin{cases} -1 & \text{if } c_j = -h_j \\ +1 & \text{otherwise} \end{cases}$$

$$\sigma_{jk}(c) = \sigma_j(c)\sigma_k(c) \tag{6.2.1}$$

and the first- and second-order partial derivative correction terms

$$D_j(f) = \sum_c \sigma_j(c)\mathcal{D}_j' f(c)$$

$$D_{jk}(f) = \sum_c \sigma_{jk}(c)\mathcal{D}_j'\mathcal{D}_k' f(c) \tag{6.2.2}$$

where the sums are over the 2^N corner points of R. Figures 6.2.1 and 6.2.2 illustrate two of the partial derivative correction terms for the 4-cube. Moreover, careful inspection will reveal the sign arrangements for $D_1(f)$ and $D_{12}(f)$ for the 2- and 3-cubes.

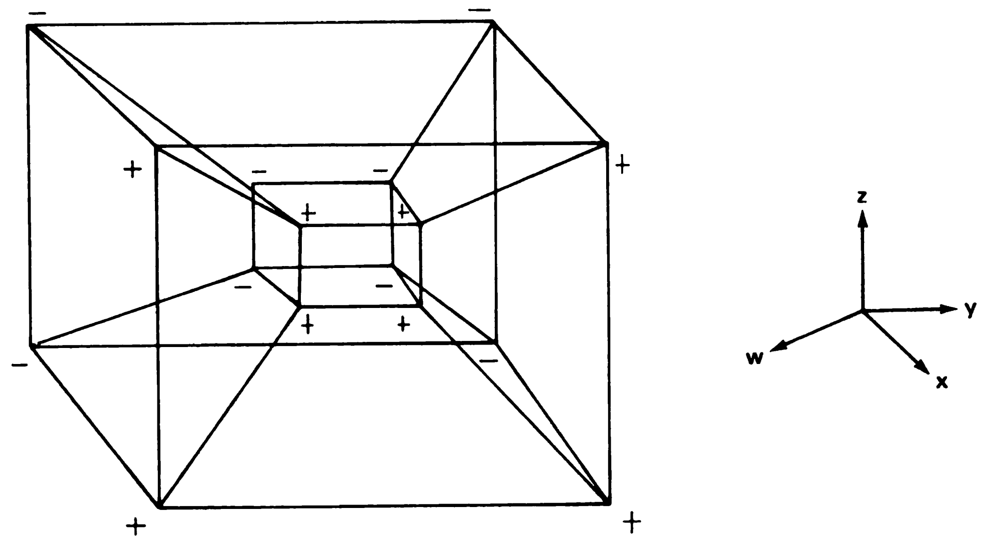


Figure 6.2.1 Sign Arrangement for $D_1(f)$

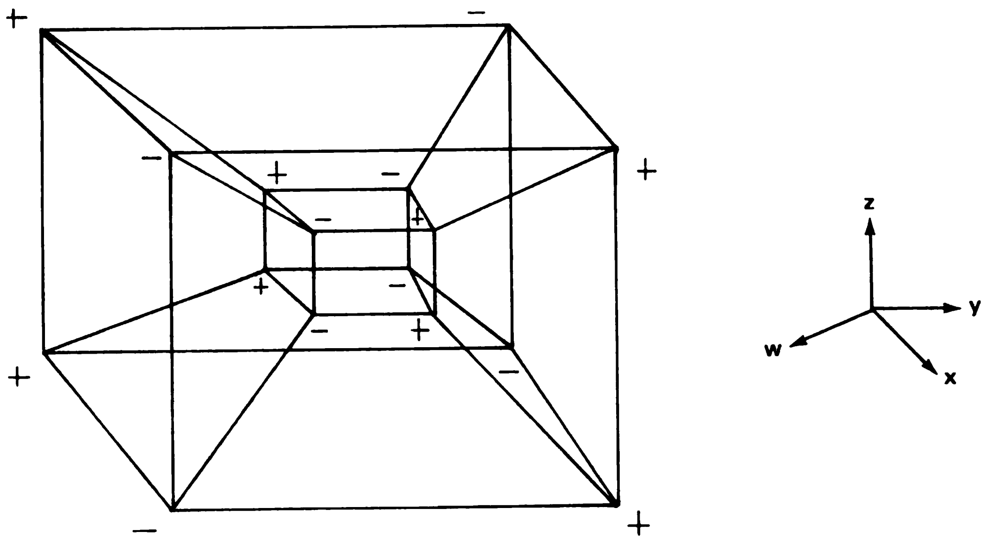


Figure 6.2.2 Sign Arrangement for $D_{12}(f)$

Since $I(f)$ and the "cubature elements"

$$A_0(f) = hf(0)$$

$$A_c(f) = h\sum_{c} f(c)$$

$$A'_c(f) = h\sum_{j=1}^{N} h_j D_j(f) \tag{6.2.3}$$

$$A''_c(f) = h\sum_{j<k} h_j h_k D_{jk}(f)$$

vanish for functions which are odd in any variable, we may approximate $I(f)$ by the linear combination

$$Q(f) = \lambda_1 A_0 + \lambda_2 A_c + \lambda_3 A'_c + \lambda_4 A''_c \tag{6.2.4}$$

which is exact for the even functions $1, x_1^2, x_1^4$, and $x_1^2 x_2^2$. By symmetry, $Q(f)$ will then also be exact for all polynomials of degree at most 5.

Now let $x = (x_1, \cdots, x_N)$ and

$$M_{jk\cdots l}^{\alpha\beta\cdots\gamma} = \max_{x\epsilon R} |\partial_l^\gamma \cdots \partial_k^\beta \partial_j^\alpha f(x)|. \tag{6.2.5}$$

Theorem 6.2.1

If $f(x_1, \cdots, x_N)$ has continuous partial derivatives of the first six orders on R, then

$$I(f) = [8A_0 + (7A_c - A'_c - A''_c/3)/2^N]/15 + E(f) \tag{6.2.6}$$

is a multidimensional quadrature formula with degree of precision 5. The truncation error. $E(f)$, is bounded by

$$|E(f)| \leqslant \frac{h}{9450}\left[\sum_{j=1}^{N} h_j^6 M_j^6 + 35 \sum_{\substack{j,k=1 \\ j\neq k}}^{N} h_j^4 h_k^2 M_{jk}^{42} + 280 \sum_{j<k<l} h_j^2 h_k^2 h_l^2 M_{jkl}^{222}\right] \tag{6.2.7}$$

Proof:

Applying Taylor's theorem for N-variables to (6.2.4) and equating coefficients of similar terms we obtain the linear system

$$\begin{bmatrix} 1 & 2^N & 0 & 0 \\ 0 & 2^{N-1} & 2^N & 0 \\ 0 & \frac{1}{3}2^{N-3} & \frac{1}{3}2^{N-1} & 0 \\ 0 & 2^{N-2} & 2^N & 2^N \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{bmatrix} = \begin{bmatrix} 1 \\ \frac{1}{6} \\ \frac{1}{120} \\ \frac{1}{36} \end{bmatrix} \tag{6.2.8}$$

having the unique solution

$$(\lambda_1, \lambda_2, \lambda_3, \lambda_4) = (8/15, 7/2^N 15, -1/2^N 15, -1/2^N 45). \tag{6.2.9}$$

The bound on the truncation error is a consequence of Taylor's theorem and is a straightforward calculation. Observe that the last term in the error appears only for $N > 2$. □

Next we transform the variables to obtain a formula for an N-fold integral over an arbitrary N-rectangle,

$$R = \prod_{j=1}^{N} [a_j, b_j].$$

Let $w_j = b_j - a_j$, $w = \prod_{j=1}^{N} w_j$, $m = (m_1, \cdots, m_N)$, and $c = (c_1, \cdots, c_N)$ where $m_j = \frac{1}{2}(a_j + b_j)$ and $c_j = a_j$ or b_j. Define

$$\sigma_j(c) = \begin{cases} -1 & \text{if } c_j = a_j \\ +1 & \text{otherwise} \end{cases}$$

$$\sigma_{jk}(c) = \sigma_j(c)\sigma_k(c). \tag{6.2.10}$$

Corollary 6.2.1

For any N-dimensional hyperrectangle, $R = \prod_{j=1}^{N} [a_j, b_j]$,

$$\int_{a_N}^{b_N} \cdots \int_{a_1}^{b_1} f(x_1, \cdots, x_N) dx_1 \cdots dx_N$$

$$= \frac{8w}{15} f(m) + \frac{7w}{2^N 15} \sum_c f(c) \tag{6.2.11}$$

$$- \frac{w}{2^{N+1} 15} \sum_{j=1}^{N} w_j D_j(f) - \frac{w}{2^{N+2} 45} \sum_{j<k} w_j w_k D_{jk}(f) + E(f)$$

where

$$|E(f)| \leq \frac{w}{604\,800} \left[\sum_{j=1}^{N} w_j^6 M_j^6 + 35 \sum_{\substack{j,k=1 \\ j \neq k}}^{N} w_j^4 w_k^2 M_{jk}^{42} + 280 \sum_{j<k<l} w_j^2 w_k^2 w_l^2 M_{jkl}^{222} \right] \tag{6.2.12}$$

Proof:

Make a linear change of variables in (6.2.7) to obtain

$$\int_{a_N}^{b_N} \cdots \int_{a_1}^{b_1} f(t_1, \cdots, t_N) dt_1 \cdots dt_N$$

$$= \int_{-h_N}^{h_N} \cdots \int_{-h_1}^{h_1} f\left(\frac{w_1}{2h_1 x_1}, \cdots, \frac{w_N}{2h_N x_N} \right) \frac{w}{h} dx_1 \cdots dx_N . \square \tag{6.2.13}$$

Finally, we obtain the composite formulation of (6.2.11). Partition each interval $[a_j, b_j]$ into n_j subintervals each of length $h_j = w_j/n_j$ and write

$$h = \prod_{j=1}^{N} h_j .$$

In order to condense notation we define

$$u(\theta) = (a_1 + h_1(i_1 - \theta), \cdots, a_N + h_N(i_N - \theta)) \tag{6.2.14}$$

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$$v(x_j) = (a_1 + i_1 h_1, \cdots, x_j, a_{j+1} + i_{j+1} h_{j+1}, \cdots, a_N + i_N h_N)$$

$$v(x_j, x_k) = (a_1 + i_1 h_1, \cdots, x_j, a_{j+1} + i_{j+1} h_{j+1}, \cdots, x_k, a_{k+1} + i_{k+1} h_{k+1}, \cdots, a_N + i_N h_N). \tag{6.2.15}$$

Furthermore

$$D_j(f(v)) = \gamma_j'[f(v(b_j)) - f(v(a_j))]$$

$$D_{jk}(f(v)) = \gamma_k'\gamma_j'[f(v(a_j, a_k)) - f(v(a_j, b_k)) - f(v(b_j, a_k)) + f(v(b_j, b_k))]. \tag{6.2.16}$$

We now state our main result.

Corollary 6.2.2 (MINTOV)

If $f(x_1, \cdots, x_N)$ has continuous partial derivatives of the first six orders on the N-rectangle

$R = \prod_{i=1}^{N} [a_i, b_i]$ then

$$\int_{a_N}^{b_N} \cdots \int_{a_1}^{b_1} f(x_1, \cdots, x_N) dx_1 \cdots dx_N$$

$$= \frac{8h}{15} \sum_{a=1}^{N} \sum_{i_a=1}^{n_a} f(u(1/2)) + \frac{7h}{2^N 15} \sum_{a=1}^{N} \sum_{i_a=0}^{n_a}{}' f(u(0))$$

$$- \frac{h}{2^{N+1} 15} \sum_{j=1}^{N} \sum_{\substack{a=1 \\ a \neq j}}^{N} \sum_{i_a=0}^{n_a}{}' h_j D_j(f(v))$$

$$- \frac{h}{2^{N+2} 45} \sum_{j<k} \sum_{\substack{a=1 \\ a \neq j,k}}^{N} \sum_{i_a=0}^{n_a}{}' h_j h_k D_{jk}(f(v)) + E(f) \tag{6.2.17}$$

is a composite multidimensional quadrature formula with first- and second-order partial derivative correction terms having degree of precision five. The primes signify the weight γ is to be assigned if the node is common to γ subregions. The truncation error, $E(f)$, is bounded by

$$|E(f)| \leqslant \frac{w}{604\,800}\left[\sum_{j=1}^{N} h_j^6 M_j^6 + 35 \sum_{\substack{j,k=1 \\ j \neq k}}^{N} h_j^4 h_k^2 M_{jk}^{42} + 280 \sum_{j<k<l} h_j^2 h_k^2 h_l^2 M_{jkl}^{222}\right] \quad (6.2.18)$$

Proof:

The proof follows by repeated use of (6.2.11). □

Note that the last term in (6.2.18) appears only for $N>2$. The 2-dimensional formulation is given in (6.4.4).

The name MINTOV (Multiple INTegration, Order V) is given to (6.2.14).

With appropriate interpretation of the corner and centroid nodes and the partial derivative correction terms, MINTOV is a nonproduct N-dimensional generalization of the composite Simpson's formula with end corrections (Lanczos, [28]:

$$\int_a^b f(x)dx = \frac{8h}{15}\sum_{i=1}^{n} f(a+h(i-½)) + \frac{7h}{30}\sum_{i=0}^{n}{}' f(a+ih)$$
$$-\frac{h^2}{60}[f'(b)-f'(a)] + \frac{b-a}{604\,800} h^6 f^6(\zeta). \quad (6.2.19)$$

As before, the prime on the summation signifies that the weight γ is to be assigned in case the node is common to γ subintervals. Also, $n = (b-a)/h$ and ζ is some point in $[a, b]$. The number of function evaluations is $2n + 3$.

It may also be stated that MINTOV is composite Ewing's formula [16, 49] with partial derivative correction terms. In the next section, a two-dimensional composite formulation of Ewing's formula is given as D0503.

The MINTOV truncation error estimate (6.2.18) is primarily of theoretical importance. It is useful for comparing MINTOV with other fifth-order multiple integration formulas. In practice it is usually not possible or at least not feasible to bound the required sixth-order partial derivatives. For example, it would be tedious to calculate and estimate the requisite sixth-order partials for the function

$$f(x,y,z) = \frac{1+w}{xyz} \sin(x)\sin(y)\sin(z)\,e^{-w} \quad (6.2.20)$$

on, say, the cube $\prod_{i=1}^{3} [0, \pi/2]$ where $w^2 = x^2 + y^2 + z^2$.

6.3 COMPARISON OF SEVERAL MULTIDIMENSIONAL QUADRATURE FORMULAS OF PRECISION FIVE

The attempt to compare various quadrature routines leads to the discovery of the absence of generally accepted standards of benchmarking techniques. Lyness and Kaganove [30] state that "any individual who constructs a routine can find some problem for which it is more efficient than an existing available routine, and with this evidence, arrange for its inclusion in the local subroutine library. Existing routines are not removed because there are other problems for which they are more efficient than the new routine."

They add that numerical experiments must play a basic role in the comparison testing and then distinguish between "battery experiments" and the "performance profile evaluation technique."

The battery experiment method requires the use of many different integrand functions, limits of integration, tolerances, and different quadrature routines. Two notable investigations were conducted by Caselleto, Pickett and Rice [12] at Purdue University, and by Kahaner [25] at Los Alamos Scientific Laboratory.

Kahaner tested 11 quadrature routines on 21 integrands using 3 error tolerances and eventually selected 3 routines based on average reliability and average speed.

Lyness and Kaganove [30] object to the technique used in these investigations on the basis of the difficulty of interpreting the results and of extracting definite conclusions, and because integrand functions which are "close" to one another were not used. Consequently, they recommend the use of the more popular performance profile evaluation technique which is described in detail in [31].

We will apply neither the battery experiment nor the performance profile technique to assess the merits of MINTOV. Instead, we will make general comparisons and conduct several numerical experiments using some definite integrals of our selection and several found in the literature.

Now we observe that the number of function evaluations, nfe, required for the d-dimensional MINTOV (6.2.14) is given by

$$\text{nfe} = \prod_{i=1}^{d} n_i + \prod_{i=1}^{d} (n_i + 1) + 2\sum_{j=1}^{d} \prod_{\substack{i=1 \\ i \neq j}}^{d} (n_i + 1) + 4\sum_{j<k} \prod_{\substack{i=1 \\ i \neq j,k}}^{d} (n_i + 1). \qquad (6.3.1)$$

Furthermore, in the case $n_i = (b_i - a_i)/h_i = n$ for all i,

$$\begin{aligned} \text{nfe} &= n^d + (n+1)^d + 2d(n+1)^{d-1} + 2d(d-1)(n+1)^{d-2} \\ &= 2n^d + \sum_{i=0}^{d-1} [2(d-i)^2 + 1]\binom{d}{i} n^i. \end{aligned} \tag{6.3.2}$$

Hereafter we refer to n as the "number of subdivisions" of R. Note that R is partitioned into n^d subregions. In (6.3.1) a partial derivative evaluation is counted the same as a function evaluation. For some integrands it may be necessary to weight the partial derivative evaluations. However, in many cases, because of persistence of form, the present enumeration technique will suffice for our purpose, namely, to size MINTOV and compare it with several well-known formulas.

Indeed, for functions such as $\ln(xyz)$ the first order partials require only about 40% of the time to evaluate the given function whereas functions similar to $\cos(x)\cos(y)\cos(z)$, $\exp(-xyz)$, $(1+x+y+z)^{-4}$, and even (6.2.18) require not more than 5% additional time to evaluate the first- and second-order partials than the original functions.

We will compare MINTOV with the fifth-order composite multidimensional quadrature formulas Lyness, Gauss, and Boole, which refer to the composite formulations of C_n:5-5 as listed in Stroud [49] and which is due to Mustard, Lyness and Blatt [37], the composite product Gauss, and the fifth-order composite product Newton-Cotes formulas, respectively.

MINTOV and Lyness are nonproduct formulas and as such might be expected to be more efficient than Gauss and Boole, as indeed they are.

The number of function evaluations for each rule is given in Table 6.3.1.

It can be shown that for $n \geqslant d$, MINTOV nfe $\leqslant C_n$: 5-5 nfe; equality holds only for $n = d = 2$. Also, for any $n > 1$ and any d, MINTOV nfe < Gauss nfe. Moreover, for all n, d, MINTOV nfe < Boole nfe. For example, for 8 partitions in 4 space, MINTOV, Lyness, Gauss, and Boole require 18 433, 43 425, 331 776, and 1 185 921 function evaluations, respectively.

Table 6.3.2 lists the number of function evaluations required by MINTOV for various subdivisions n and dimensions d.

Table 6.3.1 Number of Function Evaluations for Several Fifth-Order Formulas

Formula	nfe
MINTOV	$n^d + (n+1)^{d-2}[(n+1)^2 + 2d(n+d)]$
Lyness	$(n+1)^d + (2d+1)n^d$
Gauss	$(3n)^d$
Boole	$(4n+1)^d$

Table 6.3.2 MINTOV: Number of Function Evaluations Required for n Subdivisions in d-Dimensions

n \ d	1	2	3	4	5	6	7	8	9	10
1	5	17	57	177	513	1 409	3 713	9 473	23 553	57 345
2	7	29	125	529	2 165	8 569	32 933	123 457	453 221	1 634 713
4	11	65	399	2 481	15 399	94 721	575 759	3 456 161	20 496 519	
8	19	185	1 835	18 433	186 587	1 985 945	19 280 411			
16	35	617	10 947	195 297	3 500 163					
32	67	2 249	75 635	2 548 129						
64	131	8 585	562 899							
128	259	33 545	4 345 235							
256	515	132 617								
512	1027	527 369								

MINTOV may be sized by computing the maximum number of subdivisions n such that the number of function evaluations is less than some preassigned limit, say 10^6. This is done in Table 6.3.3 and the results indicate that compared to the techniques listed, MINTOV is substantially superior for dimensions 1-5.

Table 6.3.3 Maximum Number of Subdivisions n such that nfe $< 10^6$

Rule \ d	1	2	3	4	5	6	7	8	9	10
MINTOV	499 998	705	77	24	12	6	4	3	2	1
Lyness	–	408	49	17	9	6	4	3	3	2
Gauss	333 333	333	33	10	5	3	2	1	1	1
Boole	249 999	249	24	7	3	2	1	1	–	–

Finally, considering the speed of today's fourth-generation computers (cycle times are measured in nanoseconds), it is not unreasonable to expect a composite multidimensional quadrature formula to perform at least $n = 4$ subdivisions using, say, 10^6 function calls. With these admittedly rough but realistic guidelines, it is possible to estimate the maximum usable dimension for the formulas under consideration. The results in Table 6.3.4 indicate that the useful dimensional range for MINTOV is 1-7. Later we will show that MINTOV is particularly efficient and accurate in dimensions 2 and 3.

In particular, from Table 6.3.4 we see that if there is a requirement that a multiple quadrature formula employ at least $n = 4$ partitions (i.e., 4^d subregions), and not more than 10^6 function evaluations, then the maximum usable dimensions are 5 for Gauss and 7 for MINTOV.

Table 6.3.4 Maximum Usable Dimension d Assuming $n \geqslant 4$ and nfe $\leqslant 10^a$

Rule \ max nfe	10^2	10^3	10^4	10^5	10^6
MINTOV	2	3	4	6	7
Lyness	–	3	4	6	7
Gauss	1	2	3	4	5
Boole	1	2	3	4	4

6.4 CONSTRUCTION OF 47 NEW CUBATURE FORMULAS WITH PARTIAL DERIVATIVE CORRECTION TERMS AND ERROR ESTIMATES

In this section, for concreteness, the discussion will be limited to 2-dimensional quadrature or "cubature" formulas. We will simplify the notation whenever possible.

We wish to approximate the integral

$$I(f) = \int_c^d \int_a^b f(x,y)\,dxdy \tag{6.4.1}$$

over the rectangle $R = [a, b] \times [c, d]$ by a cubature formula $Q(f)$ which contains partial derivative correction terms.

Partition R into nm subrectangles each of size hk where $h = (b-a)/n$ and $k = (d-c)/m$. Define the following cubature elements:

$$FO = hk \sum_{j=1}^{m} \sum_{i=1}^{n} f(a + h(i - ½),\ c + k(j - ½))$$

$$FV = hk {\sum_{j=0}^{m}}' {\sum_{i=0}^{n}}' f(a + ih, c + jk)$$

$$\begin{aligned} FM = {} & hk \sum_{i=1}^{n} [f(a + h(i - ½), c) + f(a + h(i - ½), d)] \\ & + hk \sum_{j=1}^{m} [f(a, c + k(j - ½)) + f(b, c + k(j - ½))] \\ & + hk \sum_{j=1}^{m} \sum_{i=1}^{n-1} f(a + ih, c + k(j - ½)) \\ & + hk \sum_{j=1}^{m-1} \sum_{i=1}^{n} f(a + h(i - ½), c + jk) \end{aligned} \tag{6.4.2}$$

$$\begin{aligned} FV1 = {} & h^2k {\sum_{j=0}^{m}}' [f_x(b, c + jk) - f_x(a, c + jk)] \\ & + hk^2 {\sum_{i=0}^{n}}' [f_y(a + ih, d) - f_y(a + ih, c)] \end{aligned}$$

(Equation (6.4.2) continues)

$$FM1 = h^2 k \sum_{j=1}^{m}{}' [f_x(b, c+k(j-½)) - f_x(a, c+k(j-½))]$$

$$+ hk^2 \sum_{i=1}^{n}{}' [f_y(a+h(i-½), d) - f_y(a+h(i-½), c)]$$

$$FV11 = h^2k^2[f_{xy}(a,c) - f_{xy}(b,c) + f_{xy}(b,d) - f_{xy}(a,d)] \tag{6.4.2}$$

where

$$f_x = \mathcal{D}_1^1 f(x,y)$$
$$f_y = \mathcal{D}_2^1 f(x,y) \tag{6.4.3}$$
$$f_{xy} = \mathcal{D}_2^1 \mathcal{D}_1^1 f(x,y).$$

Let

$$M_{12}^{ij} = \max_{(x,y)\in R} |\mathcal{D}_2^j \mathcal{D}_1^i f(x,y)| \tag{6.4.4}$$

$$Fij = (b-a)(d-c)\ [h^i k^j M_{12}^{ij} + h^j k^i M_{12}^{ji}] = Fji.$$

The primes on the summations in (6.4.2) signify that weight σ is to be assigned if the node is common to σ subrectangles.

As in the case of MINTOV, the method of undetermined coefficients is used to construct a variety of new cubature formulas. The results are compiled in Table 6.4.1. Of the 88 combinations considered, 52 had nonvanishing determinants. Some of the unsuccessful attempts are indicated by zeros.

The significance of the entries in Table 6.4.1 may be understood by observing that formula DC5C5 is the 2-dimensional formulation of MINTOV (6.2.17):

$$\int_c^d \int_a^b f(x,y)\,dx\,dy = \frac{8}{15} FO + \frac{7}{60} FV - \frac{1}{120} FV1 - \frac{1}{720} FV11 + E(f). \tag{6.4.5}$$

$$|E(f)| \leqslant (F60 + 35\,F42)/604\,800. \tag{6.4.6}$$

The number of function evaluations is

$$\text{nfe} = 2(nm) + 3(n+m) + 9. \tag{6.4.7}$$

Table 6.4.1 Cubature Formulas

No.	Name	Elements						Error Bound					nfe		
		FO	FV	FM	FVI	FMI	FVII	F20	F40	F22	F60	F42	*nm*	*n+m*	*c*
	Midpoint														
1	E0101	1						$\frac{1}{24}$					1	0	0
–	EF140	0					0						1	0	4
2	EM143	1				$\frac{1}{24}$			$\frac{-7}{5760}$	$\frac{1}{576}$			1	2	0
3	ET183	1			$\frac{1}{48}$				$\frac{-7}{5760}$	$\frac{-5}{576}$			1	2	4
4	EX183S	1				$\frac{1}{24}$	$\frac{1}{576}$		$\frac{-7}{5760}$				1	2	4
5	EC1C3S	1			$\frac{1}{48}$		$\frac{-5}{576}$		$\frac{-7}{5760}$				1	2	8
6	ES1C3S	1			$\frac{1}{288}$	$\frac{5}{144}$			$\frac{-7}{5760}$				1	4	4
–	EH1G0	0			0	0	0						1	4	8
	Trapezoidal														
7	T0401		$\frac{1}{4}$					$\frac{-1}{12}$					1	1	1
–	TF440		0				0		0				1	1	5
8	TM443		$\frac{1}{4}$			$\frac{-1}{12}$			$\frac{1}{720}$	$\frac{-1}{72}$			1	3	1
9	TT483		$\frac{1}{4}$		$\frac{-1}{24}$				$\frac{1}{720}$	$\frac{1}{144}$			1	3	5
10	TX483S		$\frac{1}{4}$			$\frac{-1}{12}$	$\frac{-1}{72}$		$\frac{1}{720}$				1	3	5
11	TC4C3S		$\frac{1}{4}$		$\frac{-1}{24}$		$\frac{1}{144}$		$\frac{1}{720}$				1	3	9
12	TS4C3S		$\frac{1}{4}$		$\frac{-1}{36}$	$\frac{-1}{36}$			$\frac{1}{720}$				1	5	5
–	TH4G0		0		0	0	0						1	5	9
	Squire														
13	M0401			$\frac{1}{4}$				$\frac{-1}{48}$					2	1	0
–	MF440			0			0		0				2	1	4
14	MM443			$\frac{1}{4}$		$\frac{-1}{48}$			$\frac{1}{11520}$	$\frac{1}{576}$			2	3	0
15	MT483			$\frac{1}{4}$	$\frac{-1}{96}$				$\frac{1}{11520}$	$\frac{1}{144}$			2	3	4
16	MX483S			$\frac{1}{4}$		$\frac{-1}{48}$	$\frac{1}{576}$		$\frac{1}{11520}$				2	3	4
17	MC4C3S			$\frac{1}{4}$	$\frac{-1}{96}$		$\frac{1}{144}$		$\frac{1}{11520}$				2	3	8
18	MS4C3S			$\frac{1}{4}$	$\frac{1}{288}$	$\frac{-1}{36}$			$\frac{1}{11520}$				2	5	4
–	MH4G0			0	0	0	0						2	5	8
	Ewing														
19	D0503	$\frac{2}{3}$	$\frac{1}{12}$						$\frac{-1}{2880}$	$\frac{-1}{288}$			2	1	1
20	DF543S	$\frac{2}{3}$	$\frac{1}{12}$				$\frac{-1}{288}$		$\frac{-1}{2880}$				2	1	5
21	DM543A	$\frac{8}{9}$	$\frac{1}{36}$			$\frac{1}{36}$			$\frac{-1}{1080}$				2	3	1
22	DM543B	$\frac{8}{15}$	$\frac{7}{60}$			$\frac{-1}{60}$				$\frac{-1}{180}$			2	3	1
23	DT583A	$\frac{4}{9}$	$\frac{5}{36}$		$\frac{-1}{72}$				$\frac{1}{4320}$				2	3	5
24	DT583B	$\frac{8}{15}$	$\frac{7}{60}$		$\frac{-1}{120}$					$\frac{-1}{720}$			2	3	5

Table 6.4.1 (cont'd.)

No.	Name	Elements FO	FV	FM	FVI	FMI	FVII	Error Bound F20	F40	F22	F60	F42	nfe nm	n+m	c
25	DX585	$\frac{8}{15}$	$\frac{7}{60}$			$\frac{-1}{60}$	$\frac{-1}{180}$				$\frac{1}{604800}$	$\frac{7}{69120}$	2	3	5
	MINTOV														
26	DC5C5	$\frac{8}{15}$	$\frac{7}{60}$		$\frac{-1}{120}$		$\frac{-1}{720}$				$\frac{1}{604800}$	$\frac{1}{17280}$	2	3	9
27	DS5C5	$\frac{8}{15}$	$\frac{7}{60}$		$\frac{-1}{90}$	$\frac{1}{180}$					$\frac{1}{604800}$	$\frac{1}{23040}$	2	5	5
28	C5A DH5G5S	$\frac{8}{15}$	$\frac{7}{60}$		$\frac{-7}{360}$	$\frac{1}{45}$	$\frac{1}{240}$				$\frac{1}{604800}$		2	5	9
	Tyler														
29	X0503	$\frac{1}{3}$		$\frac{1}{6}$					$\frac{-1}{2880}$	$\frac{1}{576}$			3	1	0
30	XF543S	$\frac{1}{3}$		$\frac{1}{6}$			$\frac{1}{576}$		$\frac{-1}{2880}$				3	1	4
31	XM543T	$\frac{1}{15}$		$\frac{7}{30}$		$\frac{-1}{60}$				$\frac{1}{576}$			3	3	0
32	XT583A	$\frac{4}{9}$		$\frac{5}{36}$	$\frac{1}{288}$				$\frac{-17}{34560}$				3	3	4
33	XT583B	$\frac{1}{15}$		$\frac{7}{30}$	$\frac{-1}{120}$					$\frac{17}{2880}$			3	3	4
34	XX585	$\frac{1}{15}$		$\frac{7}{30}$		$\frac{-1}{60}$	$\frac{1}{576}$				$\frac{1}{604800}$	$\frac{-7}{138240}$	3	3	4
35	XC5C5	$\frac{1}{15}$		$\frac{7}{30}$	$\frac{-1}{120}$		$\frac{17}{2880}$				$\frac{1}{604800}$	$\frac{-13}{138240}$	3	3	8
36	XS5C5	$\frac{1}{15}$		$\frac{7}{30}$	$\frac{1}{288}$	$\frac{-17}{720}$					$\frac{1}{604800}$	$\frac{-1}{30720}$	3	5	4
37	XH5G5S	$\frac{1}{15}$		$\frac{7}{30}$	$\frac{7}{720}$	$\frac{-13}{360}$	$\frac{-1}{320}$				$\frac{1}{604800}$		3	5	8
	Miller														
38	O0803		$\frac{-1}{12}$	$\frac{1}{3}$					$\frac{-1}{2880}$	$\frac{1}{144}$			3	2	1
39	OF843S		$\frac{-1}{12}$	$\frac{1}{3}$			$\frac{1}{144}$		$\frac{-1}{2880}$				3	2	5
40	OM843A		$\frac{1}{36}$	$\frac{2}{9}$		$\frac{-1}{36}$			$\frac{1}{4320}$				3	4	1
41	OM843B		$\frac{-1}{60}$	$\frac{4}{15}$		$\frac{-1}{60}$				$\frac{1}{360}$			3	4	1
42	OT883T		$\frac{-1}{60}$	$\frac{4}{15}$	$\frac{-1}{120}$					$\frac{1}{144}$			3	4	5
43	OX885		$\frac{-1}{60}$	$\frac{4}{15}$		$\frac{-1}{60}$	$\frac{1}{360}$				$\frac{1}{604800}$	$\frac{-1}{13824}$	3	4	5
44	OC8C5		$\frac{-1}{60}$	$\frac{4}{15}$	$\frac{-1}{120}$		$\frac{1}{144}$				$\frac{1}{604800}$	$\frac{-1}{8640}$	3	4	9
45	OS8C5		$\frac{-1}{60}$	$\frac{4}{15}$	$\frac{1}{180}$	$\frac{-5}{180}$					$\frac{1}{604800}$	$\frac{-1}{23040}$	3	6	5
46	OH9G5S		$\frac{-1}{60}$	$\frac{4}{15}$	$\frac{5}{360}$	$\frac{-2}{45}$	$\frac{-1}{240}$				$\frac{1}{604800}$		3	6	9
	Simpson														
47	S0903S	$\frac{4}{9}$	$\frac{1}{36}$	$\frac{1}{9}$					$\frac{-1}{2880}$				4	2	1
–	SF940	0	0	0			0						4	2	5
48	SM945	$\frac{8}{45}$	$\frac{1}{36}$	$\frac{8}{45}$		$\frac{-1}{60}$					$\frac{1}{604800}$	$\frac{-1}{69120}$	4	4	1
49	ST985	$\frac{4}{9}$	$\frac{17}{180}$	$\frac{2}{45}$	$\frac{-1}{120}$						$\frac{1}{604800}$	$\frac{1}{34560}$	4	4	5
50	SX985S	$\frac{2}{9}$	$\frac{7}{180}$	$\frac{7}{45}$		$\frac{-1}{60}$	$\frac{-1}{1440}$				$\frac{1}{604800}$		4	4	5
51	SC9C5S	$\frac{16}{45}$	$\frac{13}{180}$	$\frac{4}{45}$	$\frac{-1}{120}$		$\frac{1}{720}$				$\frac{1}{604800}$		4	4	9
52	SS9C5S	$\frac{4}{15}$	$\frac{1}{20}$	$\frac{2}{15}$	$\frac{-1}{360}$	$\frac{-1}{90}$					$\frac{1}{604800}$		4	6	5
–	SH9G0	0	0	0	0	0	0						4	6	9

The first two symbols of the names assigned to the formulas listed in Table 6.4.1 were chosen somewhat arbitrarily, whereas, a digit was selected for the third symbol to represent the number of function evaluations required for the holistic or basic rule, that is for $n = m = 1$.

The fourth symbol represents the number of partial derivative evaluations required for the holistic rule. Here $C = 12$ and $G = 16$. The fifth digit is the order or degree of precision.

The presence of a sixth symbol signifies that the method of undetermined coefficients led to more equations than unknowns. The symbols A and B are used to indicate two successful combinations; whereas an S or T indicates that only one combination was successful.

For completeness, formulas 1, 7, and 47, which are the composite formulations of the midpoint, trapezoidal, and Simpson's rules, respectively, have been included. Good and Gaskins [20] recently investigated the midpoint or centroid rule. The holistic formulations of formulas 13, 19, 29, and 38 were investigated by Squire [48], Ewing [16], Tyler [51], and Miller [35] respectively. Thus except for formulas 1, 7, 13, 19, 29, 38 and 47 the remaining 45 cubature formulas are new. Formula X0503 was apparently discovered independently by Bickley [7] and Tyler [51]. We will follow Stroud [49] and call it Tyler's rule.

It is interesting to compare DF543S with Simpson's rule, S09Ø3S, because both are third-order formulas and both have the same error bounds; however, the former requires half as many function evaluations as Simpson's rule. Moreover, DF543S requires only 4 second-order mixed partial derivatives evaluated at the vertices of the rectangle R. There may be applications where DF543S should be considered as a viable alternative to Simpson's Rule.

DF543S is a combined trapezoidal-midpoint or Ewing rule [16] with boundary correction terms. This was the first cubature formula discovered which requires mixed second-order partial derivatives evaluated only at the corners of the rectangular domain of integration R. Observe that the two formulas, XF543S and OF893S, which share this property with DF543S also have the same error bound as Simpson's rule. They are also more efficient than Simpson's rule.

For smooth functions, DH5G5S will likely provide the greatest accuracy with the most economy. For brevity, we shall refer to DH5G5S simply as "C5A" (Corrected 5th-order Approximation).

Except for DF543S, XF543S, and OF843S, the derivative corrected formulas listed in Table 6.4.1 exhibit the same property as the formulas of Chapter 4; namely, the partial derivative correction terms are evaluated on the boundary as well as the vertices of R. Nevertheless, the cubature rules with boundary correction terms are more efficient than conventional formulas.

Since the nodes do not form a lattice, it follows that most of the cubature formulas in Table 6.4.1 are not product formulas.

Since the DC Simpson quadrature rule, (6.2.19), is constructed using the method of undetermined coefficients, it was conjectured that

$$\text{SH9G}\emptyset = \lambda_1 FO + \lambda_2 FV + \lambda_3 FM + \lambda_4 FV1 + \lambda_5 FM1 + \lambda_6 FV11$$

would be the product formulation of (6.2.19). However, the coefficient matrix of the resulting system

$$\begin{bmatrix} 1 & 4 & 4 & 0 & 0 & 0 \\ 0 & 4/2! & 2/2! & 4 & 2 & 0 \\ 0 & 4/4! & 2/4! & 4/3! & 2/3! & 0 \\ 0 & 4/2!2! & 0 & 8/2! & 0 & 4 \\ 0 & 4/6! & 2/6! & 4/5! & 2/5! & 0 \\ 0 & 4/4!2! & 0 & 1/2 & 0 & 4/3! \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \lambda_6 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/3! \\ 1/5! \\ 1/3!3! \\ 1/7! \\ 1/5!3! \end{bmatrix} \tag{6.4.8}$$

was singular and the attempt was unsuccessful.

A second and different derivation of the DC Simpson quadrature rule (6.2.19), employs the Euler-Maclaurin Summation formula. This was done in (3.1.9). (Recall that prior to Chapter 6, h denoted the distance between nodes, whereas here $h = (b - a)/n$ and $k = (d - c)/m$).

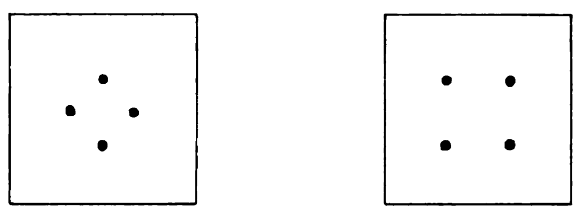
Similarly, the double Euler-Maclaurin Summation formula may be used to construct the DC Simpson cubature rule (5.2.7), which is a product formulation of (3.1.9).

The formulas in Table 6.4.1 are first-, third-, and fifth-order rules. It is somewhat disappointing that SH9G∅ did not produce a seventh-order formula. However, by selecting different nodes, several seventh-order derivative-corrected rules can be constructed. To this end, define the elements

$$FA = \sum_{j=1}^{2m}\sum_{i=1}^{n} f(a - h/2 + ih,\ c + k/4 + jk/2) + \sum_{j=1}^{m}\sum_{i=1}^{2n} f(a + h/4 + ih/2,\ c - k/2 + jk) \tag{6.4.9}$$

$$FB = \sum_{j=0}^{2m-1}\sum_{i=0}^{2n-1} f(a + h/4 + ih/2,\ c + k/4 + jk/2)$$

with nodes arranged as shown in Figure 6.4.1.



FA FB

Figure 6.4.1 Node Arrangements

Thus we have the seventh-order formulas

$$\int_c^d\int_a^b f(x,y)\,dx\,dy = -\frac{44}{105}FO + \frac{13}{420}FV + \frac{10}{189}FM + \frac{256}{945}FA - \frac{1}{504}FV1 + \frac{1}{3360}FV11 + E(f) \tag{6.4.10}$$

$$|E(f)| \leqslant (F80 + 28F62 + 364F44)/1\,625\,702\,400 \tag{6.4.11}$$

and

$$\int_c^d \int_a^b f(x,y)dxdy = \frac{4}{63}FO + \frac{61}{3780}FV + \frac{26}{315}FM$$

$$+ \frac{128}{945}FB - \frac{1}{504}FV1 + \frac{1}{1440}FV11 + E(f). \qquad (6.4.12)$$

$$|E(f)| \leqslant (F80 + 112F62 + 854F44)/1625\ 702\ 400. \qquad (6.4.13)$$

Here (6.4.10) is a derivative corrected Tyler [51] cubature rule and (6.4.12) is a derivative corrected Albrecht, Collatz [3] and Meister [34] rule. In both cases

$$\text{nfe} = 8(nm) + 4(n+m) + 9 \qquad (6.4.14)$$

which is substantially better than the $16nm$ fe required by the seventh-order composite product Gauss formula.

Finally, we note that as in the case of MINTOV, the formulas of this section can be generalized to multidimensional quadrature rules. Indeed, with appropriate generalizations of *FO*, *FV*, etc., for $N \geqslant 3$ it can be shown that

$$\int_{a_N}^{b_N} \cdots \int_{a_1}^{b_1} f(x_1, \cdots, x_N)dx_1 \cdots dx_N$$

$$= \frac{8(14-5N)}{135} FO + \frac{23}{2^N\, 135} FV + \frac{4}{27} FM$$

$$- \frac{1}{2^N\, 270} FV1 - \frac{2}{135} FM1 - \frac{1}{2^N\, 540} FV11 + E(f). \qquad (6.4.15)$$

$$|E(f)| \leqslant \frac{w}{604\ 800} \sum_{j=1}^{N} h_j^6\, M_j^6 . \qquad (6.4.16)$$

7. NUMERICAL RESULTS

7.1 DOUBLE INTEGRALS AND THE DC-MQUAD ALGORITHM

The 2-dimensional formulation of MINTOV is an accurate and efficient cubature rule. As previously noted, it requires $2(nm) + 3(n + m) + 9$ function evaluations.

Let the rectangle $R = [a, b] \times [c, d]$ be partitioned into nm subrectangles each of size $hk = (b - a)(d - c)/nm$ and let $Q(f)$ denote the approximation provided by a cubature rule.

For ease of reference the two-dimensional formulation of MINTOV is given below.

$$\int_c^d \int_a^b f(x,y)\,dx\,dy = \frac{8hk}{15} \sum_{j=1}^{m} \sum_{i=1}^{n} f(a + h(i - ½), c + k(j - ½))$$

$$+ \frac{7hk}{60} \sum_{j=0}^{m}{}' \sum_{i=0}^{n}{}' f(a + ih, c + jk) \tag{7.1.1}$$

$$- \frac{h^2k}{120} \sum_{j=0}^{m}{}' [f_x(b, c+jk) - f_x(a, c+jk)]$$

$$- \frac{hk^2}{120} \sum_{i=0}^{n}{}' [f_y(a + ih, d) - f_y(a + ih, c)]$$

$$- \frac{h^2k^2}{720} [f_{xy}(a,c) - f_{xy}(b,c) + f_{xy}(b,d) - f_{xy}(a,d)] + E(f).$$

$$|E(f)| \leqslant \frac{(b-a)(d-c)}{604\,800} [(h^6M_1^6 + k^6M_2^6) + 35(h^4k^2M_{12}^{42} + h^2k^4M_{12}^{24})]. \tag{7.1.2}$$

Mustard, Lyness, and Blatt [37] proposed a 9-point, degree 5 cubature formula which when compounded nm times requires $6nm + (n + m) + 1$ function evaluations, fe. As before, we refer to this as Lyness. This is the most efficient, non-derivative-corrected composite fifth-order cubature formula given in the literature.

The Radon [42], Albrecht, Collatz [3] 7-point, degree 5 composite formula requires $7nm$ fe. For brevity we will call it Radon's formula.

The 9-point, degree 5 composite product Gauss cubature formula requires $9nm$ fe, and the 25-point, degree 5 composite product Boole's rule when compounded nm times requires $(4n+1)(4m+1)$ fe.

Tanimoto's [50] corrected Simpson rule requires $4nm + 6(n+m) + 9$ fe. Tanimoto's rule is the only fifth-order derivative corrected cubature formula which we found in the literature.

Table 7.1.1 shows the number of function evaluations these formulas require for various subdivisions. Clearly, in this respect, MINTOV and C5A are superior to Tanimoto, Lyness, Radon, Gauss, Boole, and even Simpson's rule.

MINTOV and C5A (formulas 26 and 28, respectively, in Table 6.4.1) have been tested on a variety of integrands with many different grid sizes and have produced excellent results with respect to accuracy, computational efficiency, and economy.

The Lyness rule also performed well on the same examples; however, it required up to 3 times the number of function evaluations and was therefore much more expensive than MINTOV or C5A. Tanimoto's rule required nearly twice as many function evaluations as either MINTOV or C5A.

We now propose a new technique for cubature with error estimates called the DC-MQUAD (Derivative Corrected--Multiple Quadrature) Algorithm.

Table 7.1.1 Nfe for Various Cubature Formulas Compounded nm Times. These are Fifth-Order Formulas Except for Simpson's Rule Which is Third-Order.

$n=m$	MINTOV $2n^2+6n+9$	C5A $2n^2+10n+9$	Simpson $4n^2+4n+1$	Tanimoto $4n^2+12n+9$	Lyness $6n^2+2n+1$	Radon $7n^2$	Gauss $9n^2$	Boole $(4n+1)^2$
1	17	21	9	25	9	7	9	25
2	29	37	25	49	29	28	36	81
4	65	81	81	121	105	112	144	289
8	185	217	289	361	401	448	576	1 089
16	617	681	1 089	1 225	1 569	1 792	2 304	4 225
32	2 249	2 377	4 225	4 489	6 209	7 168	9 216	16 641
64	8 585	8 841	16 641	17 161	24 705	28 672	36 864	66 049
100	20 609	21 009	40 401	41 209	60 501	70 000	90 000	160 801

The DC-MQUAD Algorithm

1. For a given step size, compute the 4 cubature elements *FO, FV, FV*1, and *FV*11. (For 2-dimensions this requires $2nm + 3(n + m) + 9$ function evaluations.)

2. Apply the appropriate weights given in Table 6.4.1 to these cubature elements, and compute the first-order approximations, trapezoidal (T0401) and midpoint (E0101); the third-order approximations, Ewing (D0503), DF543S, and DT583A; and the fifth-order approximation MINTOV (DC5C5) (see Table 6.4.1). In the case of apparent convergence, accept MINTOV as the approximation to $I(f)$.

3. Estimate the actual and relative errors for the first five cubature rules by computing MINTOV–$Q(f)$ and [MINTOV–$Q(f)$] /MINTOV, respectively. Use MINTOV (h_2, k_2) – MINTOV (h_1, k_1) and [MINTOV (h_2, k_2)–MINTOV (h_1, k_1)] /MINTOV (h_2, k_2) to estimate the actual and relative errors for MINTOV. Here $h_2 < h_1$ and $k_2 < k_1$. Stop when the error estimate meets the preselected requirement.

4. Decrease the grid size and repeat steps 1-3.

For a sufficiently smooth function, say one having continuous partials of the first six orders, this technique provides a close error estimate which is not only practical but is also computable.

The convergence of the DC-MQUAD algorithm is guaranteed by the following theorem.

Theorem 7.1.1

If $f(x, y)$ has continuous sixth-order partial derivatives over $R = [a, b] \times [c, d]$, then

$$\lim_{\sqrt{h^2 + k^2} \to 0} \left| \text{MINTOV} - \int_c^d \int_a^b f(x,y)\,dx\,dy \right| = 0. \tag{7.1.3}$$

Proof:

Since the sixth-order partial derivatives are continuous over a compact region R, they are bounded on R. Then clearly, the truncation error is bounded by

$$|E(f)| \leqslant \frac{(b-a)(d-c)}{604\,800} \left[(h^6 M_1^6 + k^6 M_2^6) + 35(h^4 k^2 M_{12}^{42} + h^2 k^4 M_{12}^{24}) \right] \tag{7.1.4}$$

and goes to zero as $\sqrt{h^2 + k^2}$ goes to zero. □

Similar theorems can be proved for each of the formulas listed in Table 6.4.1.

Since the cubature formulas in Table 6.4.1 generalize to n-dimensions, it follows that the DC-MQUAD algorithm can be generalized for the approximation of multiple integrals of the form

$$I(f) = \int_{a_n}^{b_n} \cdots \int_{a_1}^{b_1} f(x_1, \cdots, x_n) dx_1 \cdots dx_n. \tag{7.1.5}$$

Finally we note that if the six cubature elements FO, FV, FM, $FV1$, $FM1$, and $FV11$ are computed, by using only $4nm + 6(n+m) + 9$ function evaluations, all 52 approximations to the integral $I(f)$ furnished by the cubature formulas of Table 6.4.1 may be obtained. In this connection, see Section 7.1.5 for numerical results.

Now we give the results of some numerical experiments.

7.1.1 THE APPLICATION OF MINTOV

Consider the approximation of

$$\int_0^1 \int_0^1 \frac{dxdy}{1 + x^2y^2} = \int_0^{\pi/2} \int_0^{\pi/2} \frac{dxdy}{2(1 + \cos(x)\cos(y))} = \int_0^1 \frac{\tan^{-1}(x)dx}{x} \tag{7.1.1.1}$$

$$= 0.915\,965\,594\,177\,30.$$

Taking $f(x,y) = (1 + x^2y^2)^{-1}$ and $h = k = 1/2$ in (7.1.1) we obtain

$$\begin{aligned} I(f) &\simeq \frac{8}{15}\,\frac{1}{4}\left[\frac{256}{257} + 2\left(\frac{256}{265}\right) + \frac{256}{337}\right] \\ &+ \frac{7}{60}\,\frac{1}{4}[1 + 2(1) + 1/2 + 2(2)(1) + 2(2)(4/5) + 4(16/17)] \\ &- \frac{1}{120}\,\frac{1}{8}[-1/2 - 2(8/25)](2) \end{aligned} \tag{7.1.1.2}$$

$$= \frac{169\,281\,536}{344\,270\,775} + \frac{17\,213}{40\,800} + \frac{57}{24\,000}$$

$$= 0.491\,710\,445 + 0.421\,887\,255 + 0.002\,375\,000$$

$$= 0.915\,972\,700\,0.$$

The error is 0.000 007 106 8. Here $f_x = -2xy^2(1 + x^2y^2)^{-2}$, $f_y = -2x^2y(1 + x^2y^2)^{-2}$, and $f_{xy} = 4xy(x^2y^2 - 1)(1 + x^2y^2)^{-2}$. The first-order partial derivatives f_x and f_y vanish on the axes while the second-order mixed partial derivative f_{xy} vanishes at the corners as well as on the axes.

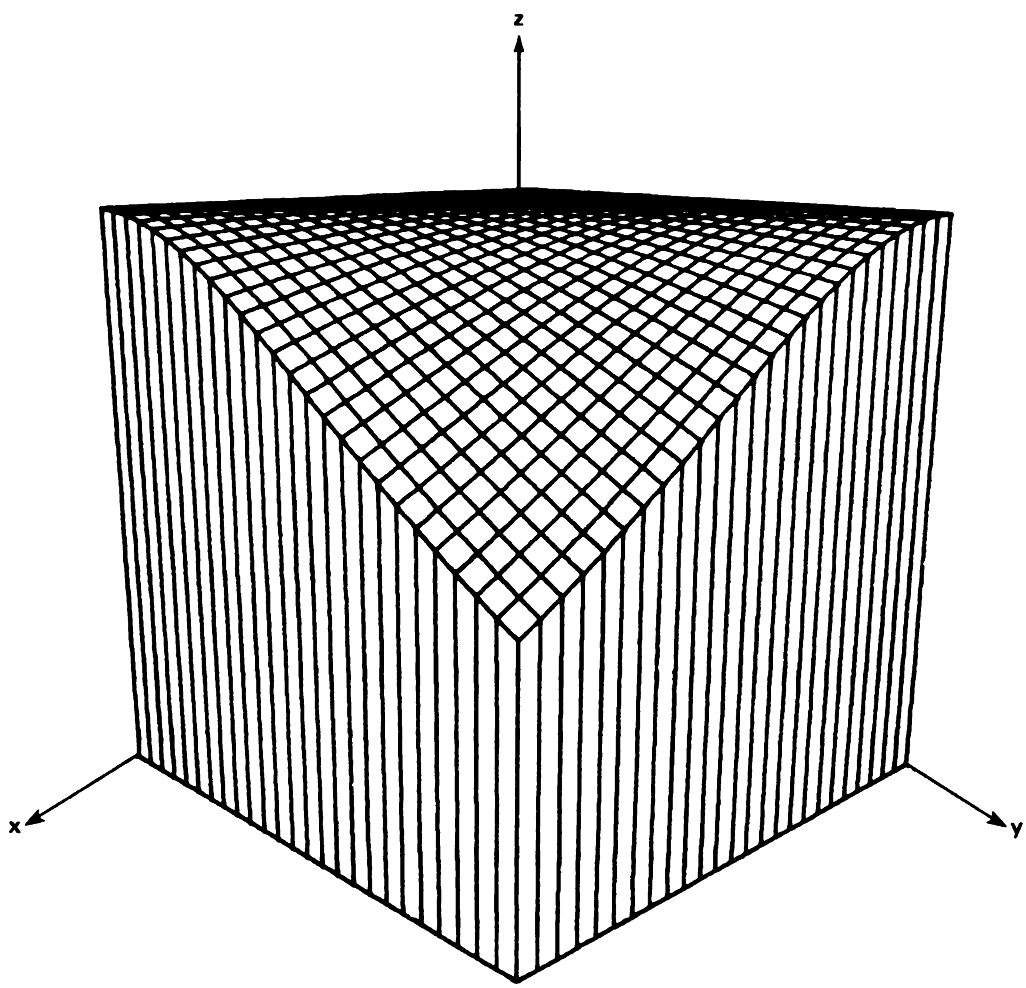


Figure 7.1.1.1 Graph of $z = (1 + x^2y^2)^{-1}$ on $[0,1]^2$

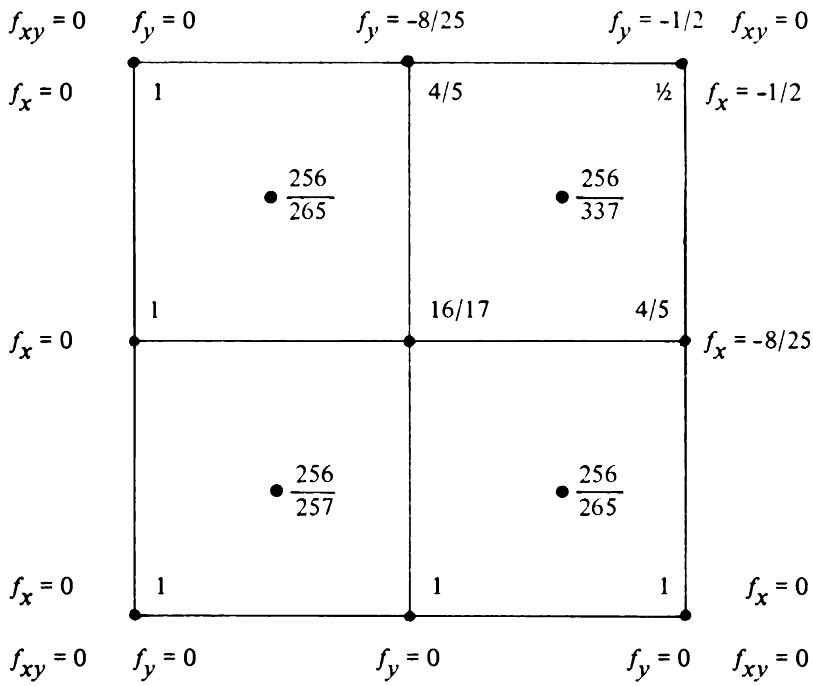


Figure 7.1.1.2 $f(x, y) = (1 + x^2y^2)^{-1}$

Figure 7.1.1.2 shows the function and partial derivative values used in the calculation (7.1.1.2). Note that the partial derivative correction terms are evaluated only on the boundary and not at interior points.

In Table 7.1.2 MINTOV is compared with several other cubature formulas.

The examples were run on the U.S. Naval Air Test Center's Real Time Telemetry Processing System Xerox Sigma 9 computer using the CPR version CØØ8 operating system and Fortran IV in double precision with 15 significant decimal digits.

Figure 7.1.1.3 shows a plot of the grid size $h = k$ vs. the logarithm of the absolute error, $\log |I(f) - Q(f)|$. The theoretical results indicate and the numerical results confirm that in terms of accuracy and economy, the derivative corrected cubature formulas provide approximations superior to comparable conventional rules.

Table 7.1.2 $\int_0^1 \int_0^1 (1 + x^2y^2)^{-1} dxdy$ = 0.915 965 594 177 30

Rule	$h = k = 1/5$ $(n = m = 5)$			$h = k = 1/10$ $(n = m = 10)$			Order†
	nfe	Time (sec)	Error	nfe	Time (sec)	Error	
Trapezoidal	36	.006	1.90-3*	121	.023	4.76-4	1
Midpoint	25	.005	-9.52-4	100	.020	-2.38-4	1
EM143	45	.015	-1.11-6	140	.039	-6.97-8	3
Ewing	61	.012	-3.44-7	221	.043	-2.04-8	3
DF543S	65	.014	-3.44-7	225	.045	-2.04-8	3
Simpson	121	.023	-3.16-7	441	.086	-1.99-8	3
MINTOV	89	.026	-2.20-8	269	.065	-3.39-10	5
C5A	109	.035	4.31-10	309	.084	8.61-12	5
SC9C5S	149	.037	5.46-10	489	.108	9.04-12	5
Tanimoto	169	.046	5.91-10	529	.128	9.22-12	5
Lyness	161	.028	5.66-9	621	.108	8.70-11	5
Radon	175	.030	-1.84-9	700	.116	-2.81-11	5
Gauss	225	.037	1.78-10	900	.145	2.83-12	5
Boole	441	.078	-1.85-10	1681	.297	-2.77-12	5

*By 1.90-3 we mean 1.90×10^{-3}

†Degree of precision

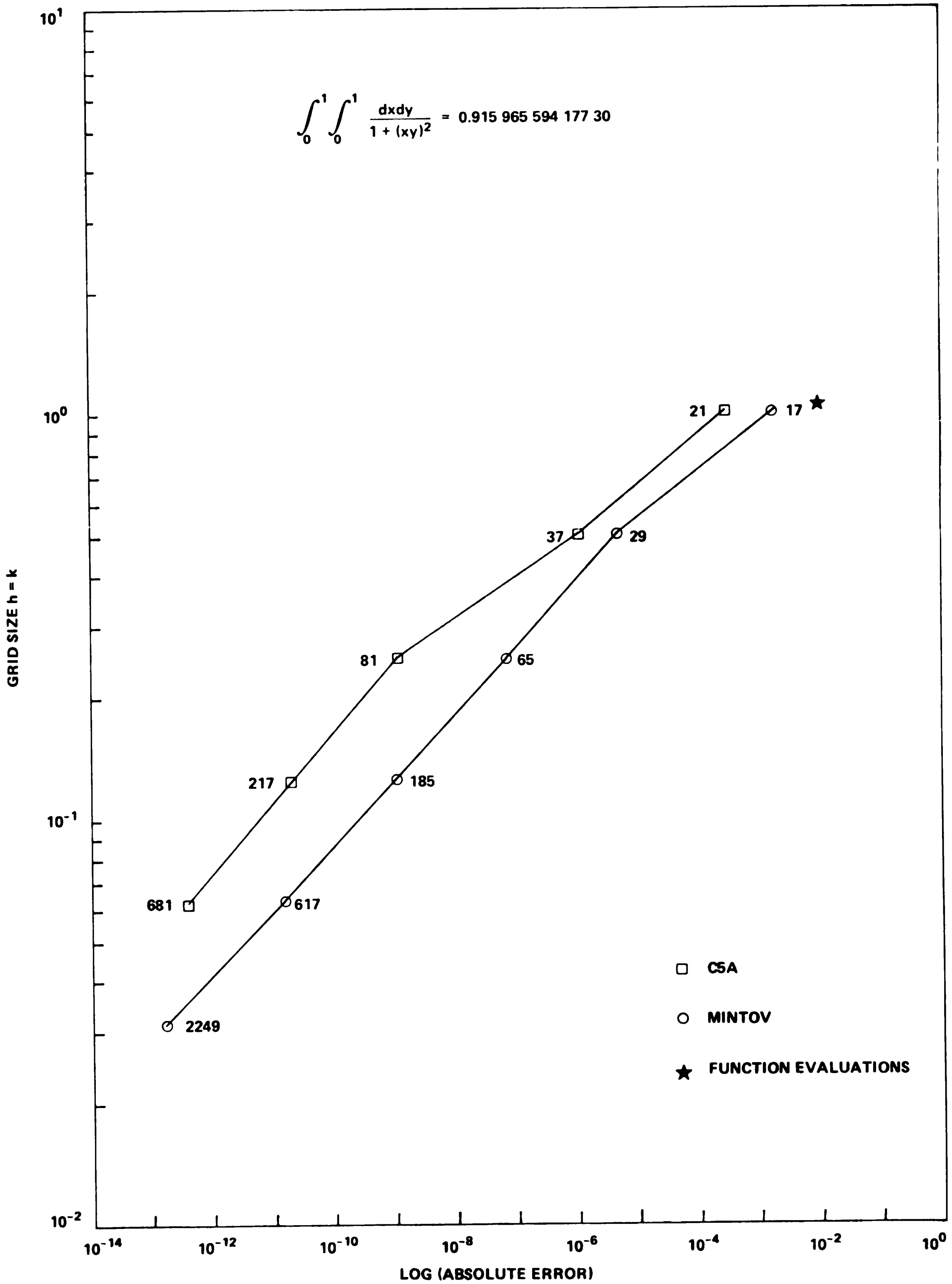


Figure 7.1.1.3 Error Curves in Approximating $\int_0^1 \int_0^1 (1 + x^2y^2)^{-1} dxdy$

7.1.2 MINTOV vs. JPL's MQUAD

Bunton, Diethelm, and Haigler [8] (hereafter referred to as Bunton) of Jet Propulsion Laboratory proposed the following example.

$$\int_1^{2.1}\int_1^{2.1} (xy)^{-1}dxdy = \ln^2(2.1) \simeq 0.550\,471\,023\,504\,079. \qquad (7.1.2.1)$$

MQUAD[1] is a Modified Romberg Multiple quadrature routine in the JPL program library. Since the single precision version computes only the first three columns of the Romberg Table, it has degree of precision 5.

Bunton states that MQUAD was designed to ". . . satisfy all the needs of a large scientific and engineering computer community. The routine is to be the 'library standard,' and its use should be greater than the total of all other special purpose quadrature routines. The standard should be one against which others could be measured. . . ."

Since both MQUAD and MINTOV are fifth-order methods, it seemed reasonable to compare them. The relative error tolerance requested for MQUAD was 10^{-4}. The grid size for MINTOV was decreased until the relative error as estimated by

$$|(\text{MINTOV}\ (h/2, k/2)\ -\ \text{MINTOV}\ (h, k))/\text{MINTOV}\ (h/2, k/2)|$$

was smaller than 10^{-4}. Under these conditions MQUAD required 441 function evaluations while MINTOV used only 65 function evaluations.

The results of MINTOV and MQUAD for a variety of relative error tolerances are presented in Table 7.1.2.1. Here MINTOV required from 1/2 to 1/26 the number of function evaluations required by the JPL routine MQUAD. Of greater significance is that MINTOV required 2% to 28% the actual computer time required by MQUAD. On the average, MINTOV is better than MQUAD by an order of magnitude.

Figures 7.1.2.1 and 7.1.2.2 show the number of function evaluations vs. absolute error for 10 different cubature formulas. For this example, SC9C5S, Tanimoto, Lyness, and Radon exhibit

[1] I am grateful to Mr. Wiley R. Bunton of JPL for sending a Fortran listing of MQUAD.

Table 7.1.2.1 MINTOV vs MQUAD for the Integral $\int_1^{2.1}\int_1^{2.1}(xy)^{-1}dxdy$ = 0.550 471 023 504 079. Relative Error Requested = 10^{-a}, a = 1(1)10.

Relative Error Requested	MINTOV			MQUAD		
	nfe	Time (sec)	Relative Error*	nfe	Time (sec)	Relative Error
10^{-1}	17	.002	1.41-3	441	.157	-1.38-7
10^{-2}	17	.002	1.41-3	441	.157	-1.38-7
10^{-3}	29	.003	3.26-5	441	.157	-1.38-7
10^{-4}	65	.010	5.91-7	441	.157	-1.38-7
10^{-5}	185	.030	9.67-9	625	.217	-3.51-8
10^{-6}	617	.100	1.53-10	1 089	.370	-4.93-9
10^{-7}	617	.100	1.53-10	2 025	.676	-3.05-10
10^{-8}	2249	.365	2.43-12	4 761	1.567	-1.19-11
10^{-9}	8585	1.395	9.41-14	15 129	4.958	-3.92-13
10^{-10}	8585	1.395	9.41-14	42 849	13.965	-3.27-14

*Relative error = $[I(f)-Q(f)]/I(f)$

approximately the same efficiency. That is, for a given number of function evaluations, they produce approximately the same absolute error.

The graphs indicate that the formulas XS5C5, C5A, and MINTOV are the most efficient cubature rules for this double integral, and MQUAD is the least efficient.

Here the Lyness truncation error is estimated by

$$|E(f)| \leqslant \frac{(b-a)(d-c)}{12\,096\,000}\left[(h^6M_1^6 + k^6M_2^6) + 175(h^4k^2M_{12}^{42} + h^2k^4M_{12}^{24})\right]. \qquad (7.1.2.2)$$

7.1.3 ERROR ESTIMATES

Stroud [49] uses the Radon-Albrecht-Collatz formula which he designates C_2:5-1 (and which we call Radon) to approximate

$$\int_{-1}^{1}\int_{-1}^{1}\sqrt{3+x+y}\,dxdy = \frac{4}{15}(1 - 18\sqrt{3} + 25\sqrt{5}) \qquad (7.1.3.1)$$

$$\approx 6.859\,942\,640\,334\,65$$

and then gives several error bounds.

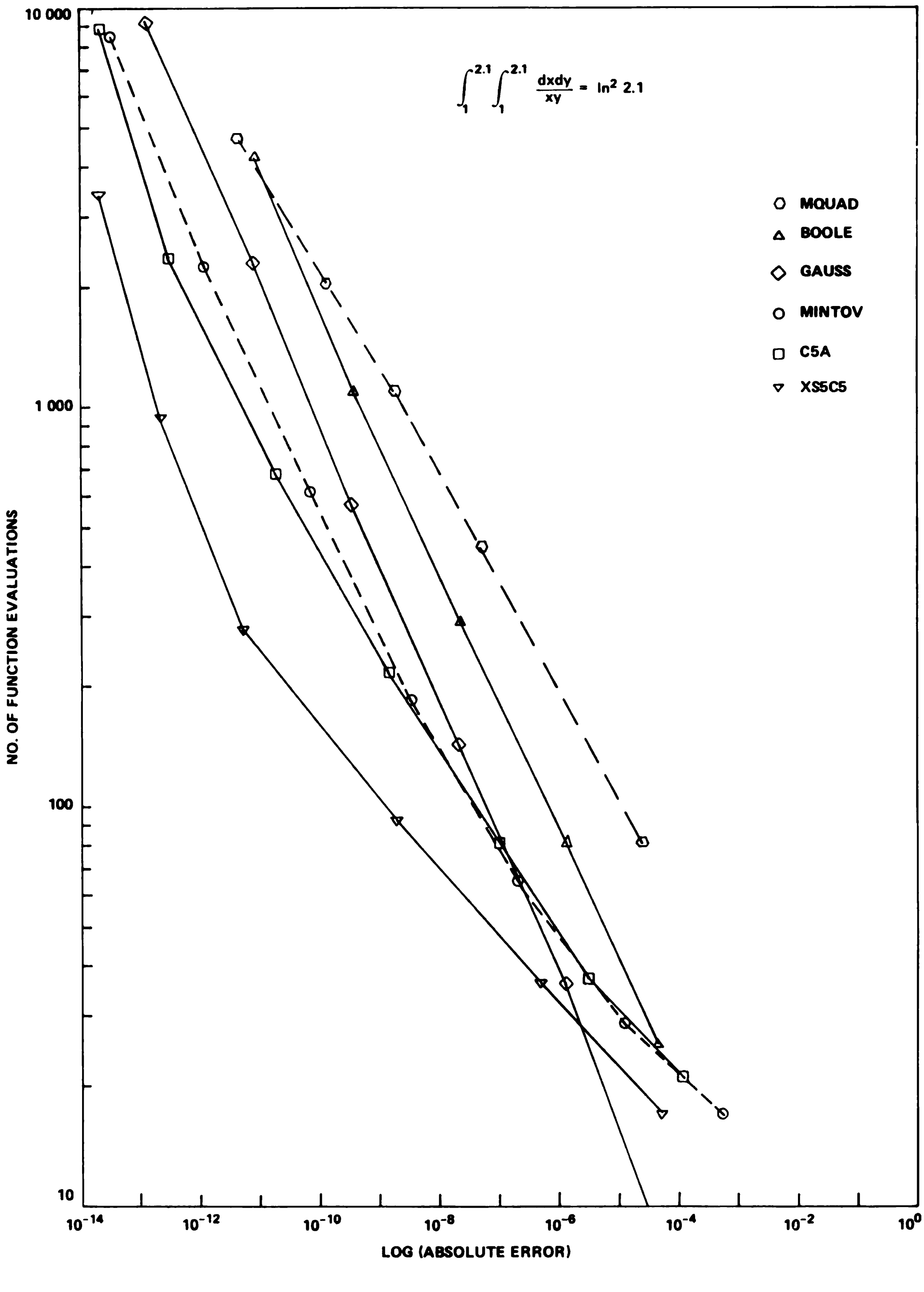


Figure 7.1.2.1 Performance Comparison in Approximating $\int_1^{2.1}\int_1^{2.1}(xy)^{-1}dxdy$

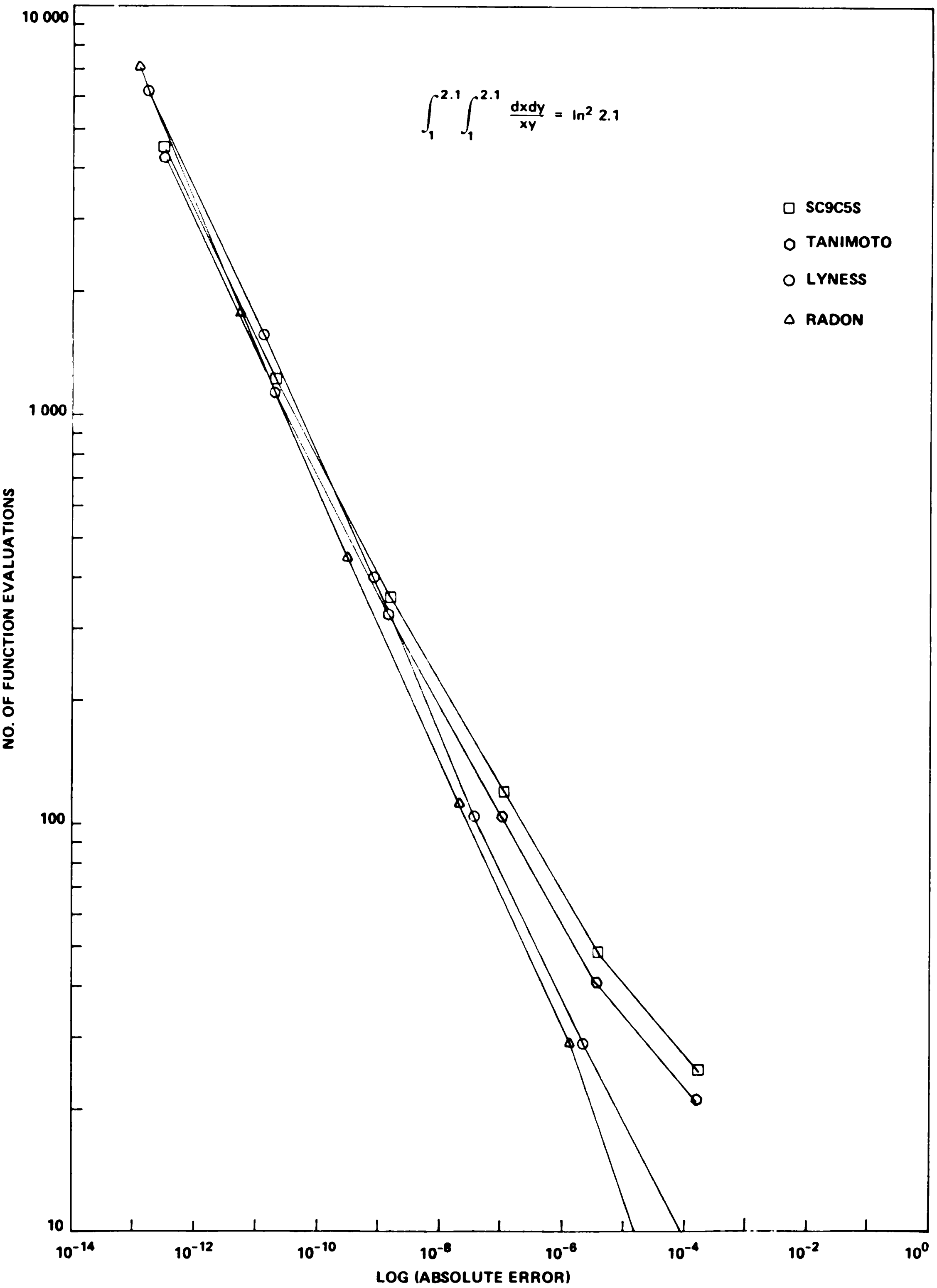


Figure 7.1.2.2 Performance Comparison in Approximating $\int_1^{2.1}\int_1^{2.1}(xy)^{-1}dxdy$

Using (7.1.2), the MINTOV truncation error estimate for this example is

$$|E(f)| \leqslant \frac{1}{10\,240}[(h^6 + k^6) + 35(h^4k^2 + h^2k^4)] \tag{7.1.3.2}$$

or in the case $h = k$

$$|E(f)| \leqslant \frac{9h^6}{1280}. \tag{7.1.3.3}$$

The results of applying various cubature formulas and error estimates to the integral (7.1.3.1) are tabulated in Table 7.1.3.1.

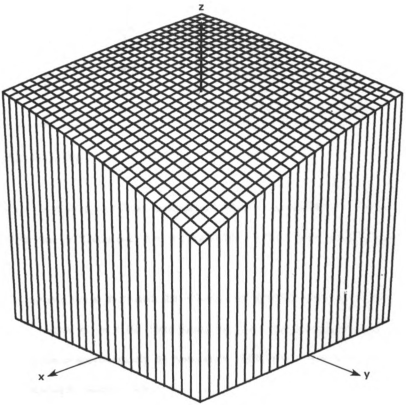


Figure 7.1.3.1 Graph of $z = \sqrt{3 + x + y}$ on $[-1, 1]^2$

Table 7.1.3.1 Error Estimates for Approximating $\int_{-1}^{1}\int_{-1}^{1} \sqrt{3+x+y}\ dxdy$ = 6.859 942 640 334 65 when $h = k = 2$ $(n = m = 1)$.

Rule	nfe	Time (sec)	Error	Error Estimate*	|Est/Err|	Order
Trapezoidal	4	.001	1.60−1	6.67−1	4	1
Midpoint	1	.000	−6.83−2	3.33−1	5	1
EM143	5	.002	7.75−4	2.50−1	323	3
Ewing	5	.001	7.75−3	2.50−1	32	3
DF543S	9	.003	−2.03−3	4.17−2	20	3
Simpson	9	.002	1.42−3	4.17−2	29	3
MINTOV	17	.007	−2.61−3	4.50−1	172	5
C5A	21	.009	7.27−4	1.25−2	17	5
SC9C5S	21	.008	1.53−4	1.25−2	81	5
Lyness	9	.002	4.51−4	1.10−1	244	5
Radon	7	.002	−1.39−4	1.48−1†	1 065	5
Radon	7	.002	−1.39−4	3.56−2†	256	5
Radon	7	.002	−1.39−4	5.73−1†	14 696	5

*See Table 6.4.1.
†Computed by Stroud [49].

At first glance, Radon appears more accurate and efficient than MINTOV. Indeed, for this example, one application of Radon does win over MINTOV. In fact, Simpson and Lyness also win over MINTOV.

However, as the grid size is decreased, the efficiency of MINTOV becomes evident. This may be seen in Table 7.1.3.2 where $n = m = 10$. Here Radon uses 2.6 times as many function evaluations as MINTOV and yet produces approximately the same error. MINTOV is now more efficient and accurate than the third-order Simpson rule.

The accuracy and efficiency of the third-order cubature formula EM143 are somewhat surprising. For $n = m = 10$, EM143 uses only 1/3 as many function evaluations as Simpson and yet produces a smaller error.

Table 7.1.3.2 Error Estimates for Approximating $\int_{-1}^{1}\int_{-1}^{1}\sqrt{3+x+y}\,dx\,dy$ = 6.859 942 640 334 65 when $h = k = 1/5$ ($n = m = 10$).

Rule	nfe	Time (sec)	Error	Error Estimate	|Est/Err|	Order
Trapezoidal	121	.029	1.52–3	6.67–3	4	1
Midpoint	100	.025	–7.59–4	3.33–3	4	1
EM143	140	.046	1.92–7	2.50–5	130	3
Ewing	221	.054	1.16–6	2.50–5	21	3
DF543S	225	.056	1.86–7	4.17–6	22	3
Simpson	441	.106	1.95–7	4.17–6	21	3
MINTOV	269	.079	–6.69–9	4.50–7	67	5
C5A	309	.100	–1.28–10	1.25–8	98	5
SC9C5S	489	.131	–1.70–10	1.25–8	74	5
Lyness	621	.136	1.62–9	1.10–7	68	5
Radon	700	.148	–5.55–10	–	–	5

The error estimates given by Stroud [49] for Radon have no provision for estimating the grid size $h \times k$ which guarantees a prescribed error. The MINTOV error estimate (7.1.3.2) as well as those given in Table 6.4.1 enjoy this advantage over those given by Stroud. Moreover, our error estimates are much easier to obtain and apply than Stroud's estimates.

Now we compute the grid size $h \times k$ which minimizes the number of function evaluations, $2(nm) + 3(n+m) + 9$, and which guarantees that the MINTOV truncation error (7.1.3.2) is smaller than 10^{-a}. The results are presented in Table 7.1.3.3.

For a function such as $g(x,y) = e^{-y}\sin(100x)$ which is changing more rapidly with respect to one variable than the other, one would take $h \ll k$.

However, in the case of (7.1.3.1), it is more convenient to set $h = k$ in (7.1.3.2). With this simplification, the MINTOV truncation error is guaranteed to be smaller than a prescribed $\varepsilon > 0$ by taking

$$n = m > 0.876\,\varepsilon^{-(1/6)}. \tag{7.1.3.4}$$

Table 7.1.3.3 $\int_{-1}^{1}\int_{-1}^{1} \sqrt{3+x+y}\,dxdy = 6.859\,942\,640\,334\,65$.

Guaranteed MINTOV Error = 10^{-a}, $a = 1(1)12$. (Grid size $h \neq k$.)

Absolute Error Guaranteed	n	m	nfe	Time (sec)	Approximation	Error	Error Estimate	|Est/Err|
10^{-1}	1	2	22	.009	6.860 473 009 882 55	-5.30-4	7.47-2	141.
10^{-2}	2	2	29	.010	6.860 014 219 003 29	-7.16-5	7.03-3	98.
10^{-3}	3	3	45	.016	6.859 950 207 911 96	-7.57-6	6.17-4	82.
10^{-4}	4	5	76	.026	6.859 943 428 653 38	-7.88-7	5.80-5	74.
10^{-5}	6	6	117	.037	6.859 942 778 121 94	-1.38-7	9.65-6	70.
10^{-6}	8	10	223	.066	6.859 942 653 717 00	-1.34-8	9.06-7	68.
10^{-7}	12	14	423	.119	6.859 942 641 780 92	-1.45-9	9.63-8	67.
10^{-8}	18	20	843	.227	6.859 942 640 481 64	-1.47-10	9.71-9	66.
10^{-9}	25	31	1 727	.450	6.859 942 640 349 67	-1.50-11	9.94-10	66.
10^{-10}	37	45	3 585	.910	6.859 942 640 336 07	-1.42-12	9.98-11	70.
10^{-11}	56	64	7 537	1.882	6.859 942 640 334 21*	4.43-13	9.88-12	22.
10^{-12}	82	94	15 953	3.936	6.859 942 640 333 46*	1.20-12	9.94-13	1.

*Contaminated by roundoff error.

The results are given in Table 7.1.3.4 and are similar to those presented in Table 7.1.3.3, except the cost of setting $h = k$ requires a few more function evaluations. In Figure 7.1.3.2, the grid size $h = k$ versus the log of the absolute error is plotted for several cubature rules.

Thus for $n = m = 41$ or $h = k \approx .05$, the actual MINTOV error is -1.35×10^{-12}. The inequality (7.1.3.3) provides a guaranteed error estimate of 9.47×10^{-11}.

Table 7.1.3.4 $\int_{-1}^{1}\int_{-1}^{1}\sqrt{3+x+y}\,dxdy$ = 6.859 942 640 334 65

Guaranteed MINTOV Error = 10^{-a}, a = 1(1)12. (Grid Size h = k.)

Absolute Error Guaranteed	$n=m$	nfe	Time (sec)	Grid Size $h=k$	Error	Error Estimate	|Est/Err|
10^{-1}	2	29	.011	1	-7.16-5	7.03-3	98
10^{-2}	2	29	.011	1	-7.16-5	7.03-3	98
10^{-3}	3	45	.016	.667	-7.57-6	6.17-4	82
10^{-4}	5	89	.030	.400	-4.01-7	2.88-5	72
10^{-5}	6	117	.037	.333	-1.38-7	9.65-6	70
10^{-6}	9	225	.068	.222	-1.25-8	8.47-7	68
10^{-7}	13	425	.120	.154	-1.40-9	9.32-8	67
10^{-8}	19	845	.227	.105	-1.45-10	9.57-9	66
10^{-9}	28	1 745	.456	.0714	-1.41-11	9.34-10	66
10^{-10}	41	3 617	.919	.0488	-1.35-12	9.47-11	70
10^{-11}	60	7 569	1.890	.0333	4.66-13*	9.65-12	21
10^{-12}	88	16 025	3.956	.0227	1.22-12*	9.69-13	1

*Accuracy affected by machine limitation of 15 significant digits.

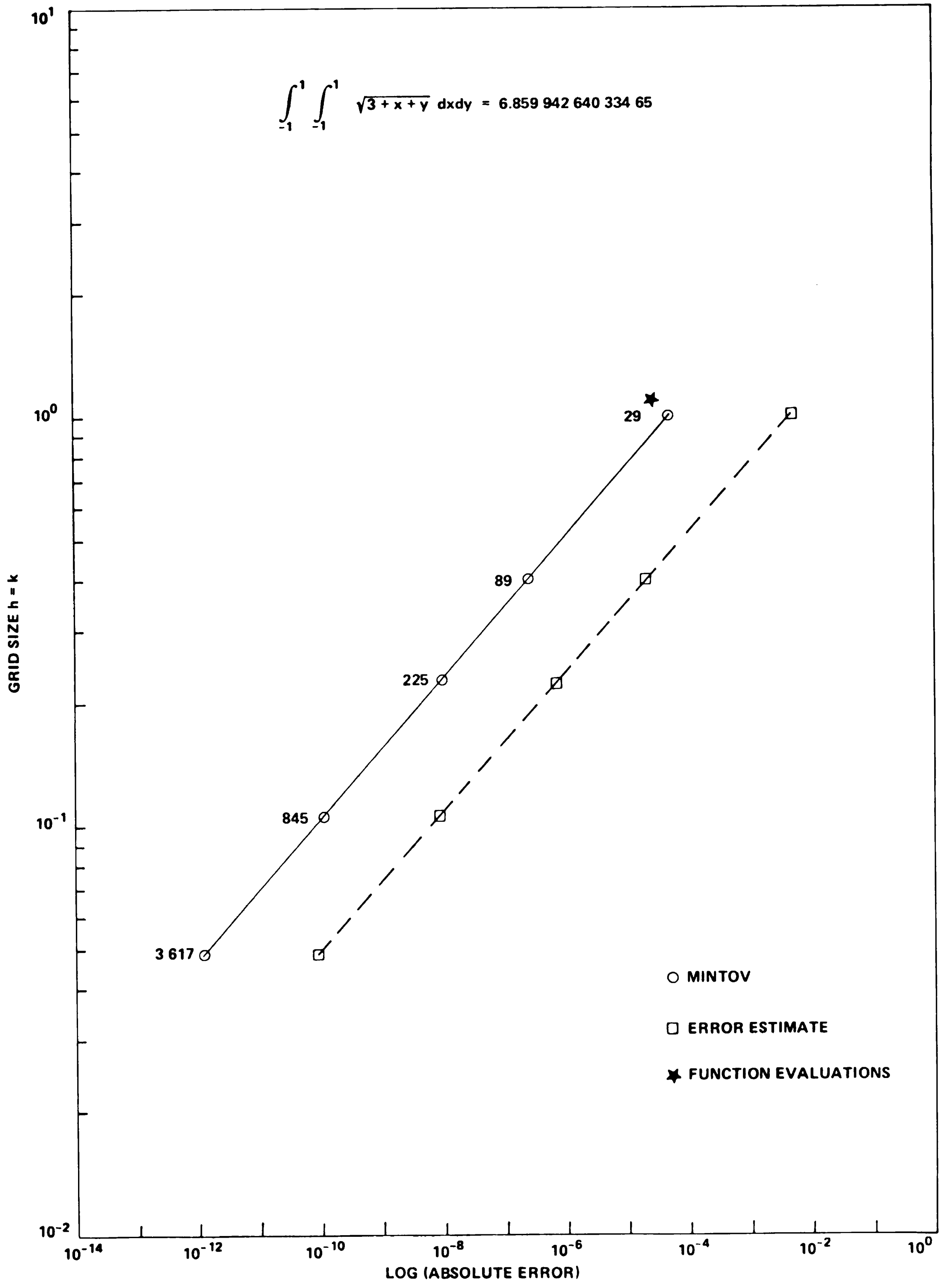


Figure 7.1.3.2 Error Curves in Approximating $\int_{-1}^{1}\int_{-1}^{1} \sqrt{3+x+y}\; dxdy$

7.1.4 A RATIONAL FUNCTION WITH A SINGULARITY APPROACHING THE DOMAIN OF INTEGRATION

Consider the double integral

$$\int_{-1}^{1}\int_{-1}^{1} \frac{dxdy}{4(w+2+x+y)} = \begin{cases} \frac{1}{4}\left[(w+4)\ln(w+4) - 2(w+2)\ln(w+2) + w\ln(w)\right], & w > 0 \\ \ln(2) \text{ (Cauchy Principal Value)}, & w = 0. \end{cases} \qquad (7.1.4.1)$$

The errors obtained when various cubature formulas are applied to this integral with $h = k = 1/50$ or $n = m = 100$ as the parameter w takes on the values 1, .5, .1, .05, .01, .001, and 0 are given in Table 7.1.4.1. Squire and the derivative corrected formula, EM143, perform quite well as w approaches 0. Simpson, Tanimoto, Lyness, Radon, Gauss, and Boole require too many function evaluations for the error returned.

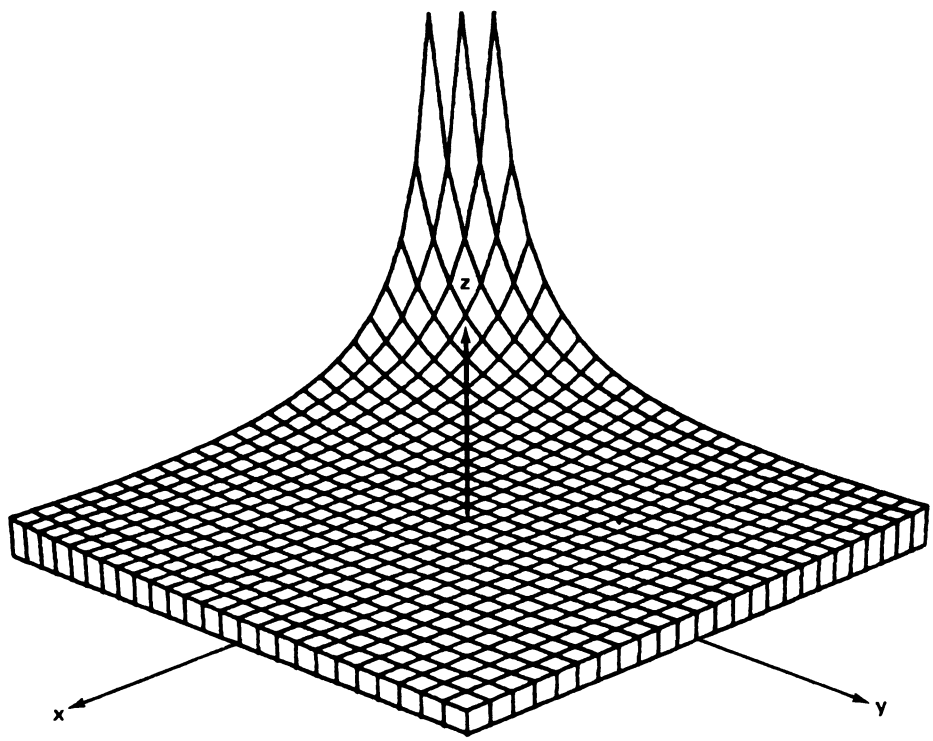


Figure 7.1.4.1 Graph of $z = \frac{1}{4}(2+x+y)^{-1}$ on $(-1,1]^2$

Table 7.1.4.1 Application of Various Cubature Formulas to $\int_{-1}^{1}\int_{-1}^{1}[4(w+2+x+y)]^{-1}dxdy$ with $h = k = 1/50$ ($n = m = 100$).

Rule	nfe	Avg Time (sec)	w: 1.0	w: 0.1	w: 0.01	w: 0.001	w: 0.0	Order
Trapezoidal	10 201	1.755	-8.89-6	-1.55-4	-1.81-3	-2.31-2	*	1
Midpoint	10 000	1.771	4.44-6	7.71-5	6.70-4	1.87-3	2.49-3	1
EM143	10 400	1.976	-5.18-11	-5.32-8	-9.48-6	1.25-4	4.44-4	3
Squire	20 200	3.491	-2.22-6	-3.84-5	-2.87-4	-3.12-4	3.12-6	3
MM443	20 600	3.696	1.43-10	1.49-7	5.29-5	5.60-4	1.03-3	3
Ewing	20 201	3.527	-3.11-10	-3.27-7	-1.57-4	-6.46-3	*	3
DF543S	20 205	3.529	-5.17-11	-4.94-8	1.20-4	2.71-1	*	3
DM543A	20 601	3.731	-1.38-10	-1.45-7	-5.88-5	-2.07-3	*	3
Tyler	30 200	5.263	7.79-11	8.14-8	3.21-5	4.15-4	8.33-4	3
XM543T	30 600	5.468	1.30-10	1.35-7	4.87-5	5.31-4	9.89-4	3
Miller	30 401	5.247	4.67-10	4.90-7	2.22-4	7.29-3	*	3
Simpson	40 401	7.019	-5.18-11	-5.48-8	-3.11-5	-1.88-3	*	3
MINTOV	20 609	3.735	1.26-13	4.37-9	1.09-4	1.35-1	*	5
C5A	21 009	3.940	8.21-14	5.25-11	-4.83-5	-2.66-1	*	5
SC9C5S	40 809	7.227	8.28-14	1.03-10	-1.17-5	-8.36-2	*	5
Tanimoto	41 209	7.390	8.41-14	1.23-10	3.00-6	-1.08-2	*	5
Lyness	60 201	9.140	1.06-14	-1.05-9	-1.55-5	-1.78-3	*	5
Radon	70 000	10.034	5.06-14	3.59-10	4.43-6	1.84-4	5.09-4	5
Gauss	90 000	12.458	3.92-14	3.68-11	8.44-7	8.71-5	3.38-4	5
Boole	160 801	24.881	4.95-14	-3.79-11	-9.66-7	-2.73-4	*	5

*Cubature rule not applicable due to singularity at (-1, -1) when $w = 0$

7.1.5 THE COMPARISON OF 45 NEW CUBATURE FORMULAS WITH 12 CONVENTIONAL RULES

In this example we present the results of applying each of the 52 cubature formulas listed in Table 6.4.1 to the integral

$$\int_0^1\int_0^1 \tfrac{1}{2}(e^x + 1)\sin(\pi y)dxdy = e/\pi. \qquad (7.1.5.1)$$

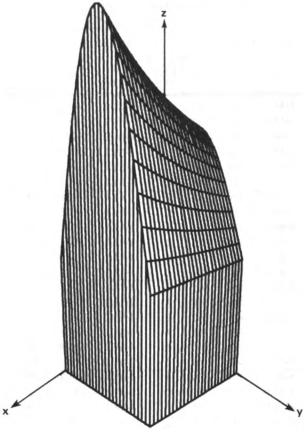


Figure 7.1.5.1 Graph of $z = \frac{1}{2}(e^x + 1)\sin(\pi y)$ on $[0, 1]^2$

For the sake of comparison, several additional cubature formulas are included. Error estimates are also provided.

The approximations were computed by a single computer program which contained a subroutine to calculate the 6 cubature elements, *FO, FV, FM, FV*1, *FM*1, *FV*11, using $4nm + 6(n + m) + 9$ fe. The cubature elements were then combined as indicated in Table 6.4.1 to produce the 52 approximations to $I(f)$. The results are tabulated in Table 7.1.5.1.

For comparison we include the results of 5 additional fifth-order cubature formulas: Tanimoto, Lyness, Radon, Gauss, and Boole.

Table 7.1.5.1 The Comparison of 45 New Cubature Formulas with 12 Conventional Rules for the Double Integral $\int_0^1 \int_0^1 \frac{1}{2}(e^x + 1)\sin(\pi y)dxdy = e/\pi$

No*	Rule	$h = k = 1$ $(n = m = 1)$					$h = k = 1/10$ $(n = m = 10)$					Order
		nfe	Time (sec)	Error	Error Estimate*	|Est/Err|	nfe	Time (sec)	Error	Error Estimate*	|Est/Err|	
1	Midpoint	1	.000	-4.59-1	8.21-1	2	100	.047	-3.34-3	8.21-3	2	1
2	EM143	5	.002	-1.48-1	2.45-1	2	140	.063	-1.13-5	2.45-5	2	3
3	ET183	9	.003	-8.48-2	3.38-1	4	144	.065	-5.64-6	3.38-5	6	3
4	EX183S	9	.003	-1.39-1	2.22-1	2	144	.065	-1.03-5	2.22-5	2	3
5	EC1C3S	13	.004	-1.32-1	2.22-1	2	148	.066	-1.03-5	2.22-5	2	3
6	ES1C3S	13	.005	-1.38-1	2.22-1	2	184	.081	-1.03-5	2.22-5	2	3
7	Trapezoidal	4	.001	8.65-1	1.64	2	121	.054	6.68-3	1.64-2	2	1
8	TM443	8	.002	2.43-1	4.40-1	2	161	.070	1.93-5	4.40-5	2	3
9	TT483	12	.004	1.17-1	3.47-1	3	165	.071	8.06-6	3.47-5	4	3
10	TX483S	12	.003	1.68-1	2.53-1	2	165	.071	1.18-5	2.53-5	2	3
11	TC4C3S	16	.005	1.54-1	2.53-1	2	169	.073	1.18-5	2.53-5	2	3
12	TS4C3S	16	.005	1.59-1	2.53-1	2	205	.087	1.18-5	2.53-5	2	3
13	Squire	4	.001	1.50-1	4.11-1	3	220	.100	1.66-3	4.11-3	2	1
14	MM443	8	.003	-4.99-3	3.91-2	8	260	.116	-2.03-7	3.91-6	19	3
15	MT483	12	.004	-3.67-2	1.09-1	3	264	.118	-3.02-6	1.09-5	4	3
16	MX483S	12	.004	4.38-3	1.58-2	4	264	.118	7.34-7	1.58-6	2	3
17	MC4C3S	16	.005	8.28-4	1.58-2	19	268	.119	7.32-7	1.58-6	2	3
18	MS4C3S	16	.006	5.57-3	1.58-2	3	304	.134	7.35-7	1.58-6	2	3
19	Ewing	5	.001	-1.77-2	1.10-1	6	221	.101	-1.08-6	1.10-5	10	3
20	DF543S	9	.002	-3.64-2	6.34-2	2	225	.103	-2.95-6	6.34-6	2	3
21	DM543A	9	.003	-1.05-1	1.69-1	2	261	.117	-7.87-6	1.69-5	2	3
22	DM543B	9	.003	3.46-2	7.45-2	2	261	.117	3.00-6	7.45-6	2	3
23	DT583A	13	.004	2.71-2	4.22-2	2	265	.119	1.97-6	4.22-6	2	3
24	DT583B	13	.004	9.23-3	1.86-2	2	265	.119	7.51-7	1.86-6	2	3
25	DX585	13	.004	4.57-3	1.77-2	4	265	.119	3.48-9	1.77-8	5	5
26	MINTOV	17	.005	1.73-3	1.14-2	7	269	.120	1.40-9	1.14-8	8	5
27	DS5C5	17	.006	7.81-4	9.29-3	12	305	.135	7.04-10	9.29-9	13	5
28	C5A	21	.007	-2.06-3	2.96-3	1	309	.136	-1.38-9	2.96-9	2	5
29	Tyler	5	.002	-5.27-2	8.66-2	2	320	.148	-3.89-6	8.66-6	2	3
30	XF543S	9	.003	-4.33-2	6.34-2	2	324	.149	-2.96-6	6.34-6	2	3
31	XM543T	9	.003	-1.45-2	2.33-2	2	360	.164	-9.41-7	2.33-6	2	3
32	XT583A	13	.005	-5.81-2	8.97-2	2	364	.165	-4.19-6	8.97-6	2	3
33	XT583B	13	.005	-3.99-2	7.92-2	2	364	.165	-3.19-6	7.92-6	2	3
34	XX585	13	.004	-5.16-3	1.03-2	2	364	.165	-3.81-9	1.03-8	3	5
35	XC5C5	17	.006	-8.01-3	1.67-2	2	368	.167	-5.89-9	1.67-8	3	5
36	XS5C5	17	.006	-3.98-3	7.70-3	2	404	.181	-2.94-9	7.70-9	3	5
37	XH5G5S	21	.007	-1.85-3	2.96-3	2	408	.183	-1.38-9	2.96-9	2	5

*See Table 6.4.1

Table 7.1.5.1 (cont'd.)

No*	Rule	$h = k = 1$ $(n = m = 1)$ nfe	Time (sec)	Error	Error Estimate*	|Est/Err|	$h = k = 1/10$ $(n = m = 10)$ nfe	Time (sec)	Error	Error Estimate*	|Est/Err|	Order
38	Miller	8	.002	-8.78-2	1.57-1	2	341	.154	-6.71-6	1.57-5	2	3
39	OF843S	12	.003	-5.03-2	6.34-2	1	345	.156	-2.96-6	6.34-6	2	3
40	OM843A	12	.004	2.26-2	4.22-2	2	381	.170	1.97-6	4.22-6	2	3
41	OM843B	12	.004	-2.15-2	3.73-2	2	381	.170	-1.50-6	3.73-6	2	3
42	OT883T	16	.005	-4.69-2	9.32-2	2	385	.172	-3.76-6	9.32-6	2	3
43	OX885	16	.005	-6.55-3	1.35-2	2	385	.172	-4.85-9	1.35-8	3	5
44	OC8C5	20	.006	-9.40-3	1.98-2	2	389	.173	-6.93-9	1.98-8	3	5
45	OS8C5	20	.007	-4.66-3	9.29-3	2	425	.188	-3.46-9	9.29-9	3	5
46	OH9G5S	24	.008	-1.81-3	2.96-3	2	429	.189	-1.38-9	2.96-9	2	5
47	Simpson	9	.003	-4.10-2	6.34-2	2	441	.202	-2.95-6	6.34-6	2	3
48	SM945	13	.004	-2.85-3	5.07-3	2	481	.213	-2.07-9	5.07-9	2	5
49	ST985	17	.006	-1.26-4	7.18-3	57	485	.219	9.91-12	7.18-9	724	5
50	SX985S	17	.005	-1.92-3	2.96-3	2	485	.219	-1.38-9	2.96-9	2	5
51	SC9C5S	21	.007	-1.98-3	2.96-3	1	489	.221	-1.38-9	2.96-9	2	5
52	SS9C5S	21	.007	-1.94-3	2.96-3	2	525	.235	-1.38-9	2.96-9	2	5
53	Tanimoto	25	.010	-1.95-3	–	–	529	.236	-1.38-9	–	–	5
54	Lyness	9	.004	-8.60-4	2.26-3	3	621	.272	-6.26-10	2.26-9	4	5
55	Radon	7	.003	8.79-4	–	–	700	.303	6.38-10	–	–	5
56	Gauss	9	.004	-6.01-4	–	–	900	.385	-4.14-10	–	–	5
57	Boole	25	.010	6.18-4	–	–	1681	.739	4.31-10	–	–	5

*See Table 6.4.1

These results are included in the sense of a benchmark test to reveal possible errors in the cubature formulas of Table 6.4.1. These and other results confirm the accuracy of the entries in Table 6.4.1.

Finally, we observe that for the double integrals considered, for any reasonable grid size the composite fifth-order cubature rules, C5A, Tanimoto, Lyness, Radon, Gauss, and Boole generally all produced approximately the same error; however, C5A required far less function evaluations and thus is the best fifth-order method.

Similar comparisons can be made for the powerful third-order derivative corrected rule EM143.

7.2 TRIPLE INTEGRALS

Denoting the step size in each dimension by $h_i = (b_i - a_i)/n_i$, $i = 1(1)3$, the 3-dimensional formulation of MINTOV is

$$
\begin{aligned}
&\int_{a_3}^{b_3}\int_{a_2}^{b_2}\int_{a_1}^{b_1} f(x,y,z)\,\mathrm{dx\,dy\,dz} \\
&= \frac{8}{15}h_1h_2h_3\sum_{i_3=1}^{n_3}\sum_{i_2=1}^{n_2}\sum_{i_1=1}^{n_1} f(a_1+h_1(i_1-½),a_2+h_2(i_2-½),a_3+h_3(i_3-½)) \\
&+ \frac{7}{120}h_1h_2h_3\sum_{i_3=0}^{n_3}{}'\sum_{i_2=0}^{n_2}{}'\sum_{i_1=0}^{n_1}{}' f(a_1+i_1h_1,\, a_2+i_2h_2,\, a_3+i_3h_3) \\
&- \frac{1}{240}h_1^2h_2h_3\sum_{i_3=0}^{n_3}{}'\sum_{i_2=0}^{n_2}{}'\,[f_x(b_1,a_2+i_2h_2,a_3+i_3h_3) \\
&\qquad - f_x(a_1,a_2+i_2h_2,a_3+i_3h_3)] \\
&- \frac{1}{240}h_1h_2^2h_3\sum_{i_3=0}^{n_3}{}'\sum_{i_1=0}^{n_1}{}'\,[f_y(a_1+i_1h_1,b_2,a_3+i_3h_3) \\
&\qquad - f_y(a_1+i_1h_1,a_2,a_3+i_3h_3)] \qquad\qquad (7.2.1) \\
&- \frac{1}{240}h_1h_2h_3^2\sum_{i_2=0}^{n_2}{}'\sum_{i_1=0}^{n_1}{}'\,[f_z(a_1+i_1h_1,a_2+i_2h_2,b_3) \\
&\qquad - f_z(a_1+i_1h_1,a_2+i_2h_2,a_3)] \\
&- \frac{1}{1440}h_1^2h_2^2h_3\sum_{i_3=0}^{n_3}{}'\,[f_{xy}(a_1,a_2,a_3+i_3h_3) - f_{xy}(a_1,b_2,a_3+i_3h_3) \\
&\qquad - f_{xy}(b_1,a_2,a_3+i_3h_3) + f_{xy}(b_1,b_2,a_3+i_3h_3)] \\
&- \frac{1}{1440}h_1^2h_2h_3^2\sum_{i_2=0}^{n_2}{}'\,[f_{xz}(a_1,a_2+i_2h_2,a_3) - f_{xz}(a_1,a_2+i_2h_2,b_3) \\
&\qquad - f_{xz}(b_1,a_2+i_2h_2,a_3) + f_{xz}(b_1,a_2+i_2h_2,b_3)] \\
&- \frac{1}{1440}h_1h_2^2h_3^2\sum_{i_1=0}^{n_1}{}'\,[f_{yz}(a_1+i_1h_1,a_2,a_3) - f_{yz}(a_1+i_1h_1,a_2,b_3) \\
&\qquad - f_{yz}(a_1+i_1h_1,b_2,a_3) + f_{yz}(a_1+i_1h_1,b_2,b_3)] + E(f).
\end{aligned}
$$

The truncation error may be estimated by

$$|E(f)| \leqslant \frac{(b_1 - a_1)(b_2 - a_2)(b_3 - a_3)}{604\ 800} \Big[(h_1^6 M_1^6 + h_2^6 M_2^6 + h_3^6 M_3^6) + 35(h_1^4 h_2^2 M_{12}^{42} + h_1^2 h_2^4 M_{12}^{24} + h_1^4 h_3^2 M_{13}^{42} + h_1^2 h_3^4 M_{13}^{24} + h_2^4 h_3^2 M_{23}^{42} + h_2^2 h_3^4 M_{23}^{24}) + 280 h_1^2 h_2^2 h_3^2 M_{123}^{222} \Big] \tag{7.2.2}$$

Table 7.2.1 lists the number of function evaluations required by various composite multiple quadrature formulas. In this respect, MINTOV is superior to the conventional formulas.

Table 7.2.1 Nfe for Several Multiple Quadrature Formulas Repeated $n_1 n_2 n_3$ Times

$n_1 = n_2 = n_3$	MINTOV $2n^3 + 9n^2 + 27n + 19$	Simpson $(2n+1)^3$	Lyness $(n+1)^3 + 7n^3$	Gauss $(3n)^3$	Boole $(4n+1)^3$
1	57	27	15	27	64
2	125	125	83	216	729
4	399	729	573	1 728	4 913
8	1 835	4 913	4 313	13 824	35 937
16	10 947	35 937	33 585	110 592	274 625
32	75 635	274 625	265 313	884 736	2 146 689
64	562 899	2 146 689	2 109 633	7 077 888	16 974 593
100	2 092 719	8 120 601	8 030 301	27 000 000	64 481 201

7.2.1 A FUNCTION WITH VANISHING MIXED HIGHER-ORDER PARTIAL DERIVATIVES

We wish to approximate the triple integral

$$\int_1^2 \int_1^2 \int_1^2 \ln(xyz)\,dx\,dy\,dz = \ln 64 - 3. \tag{7.2.1.1}$$

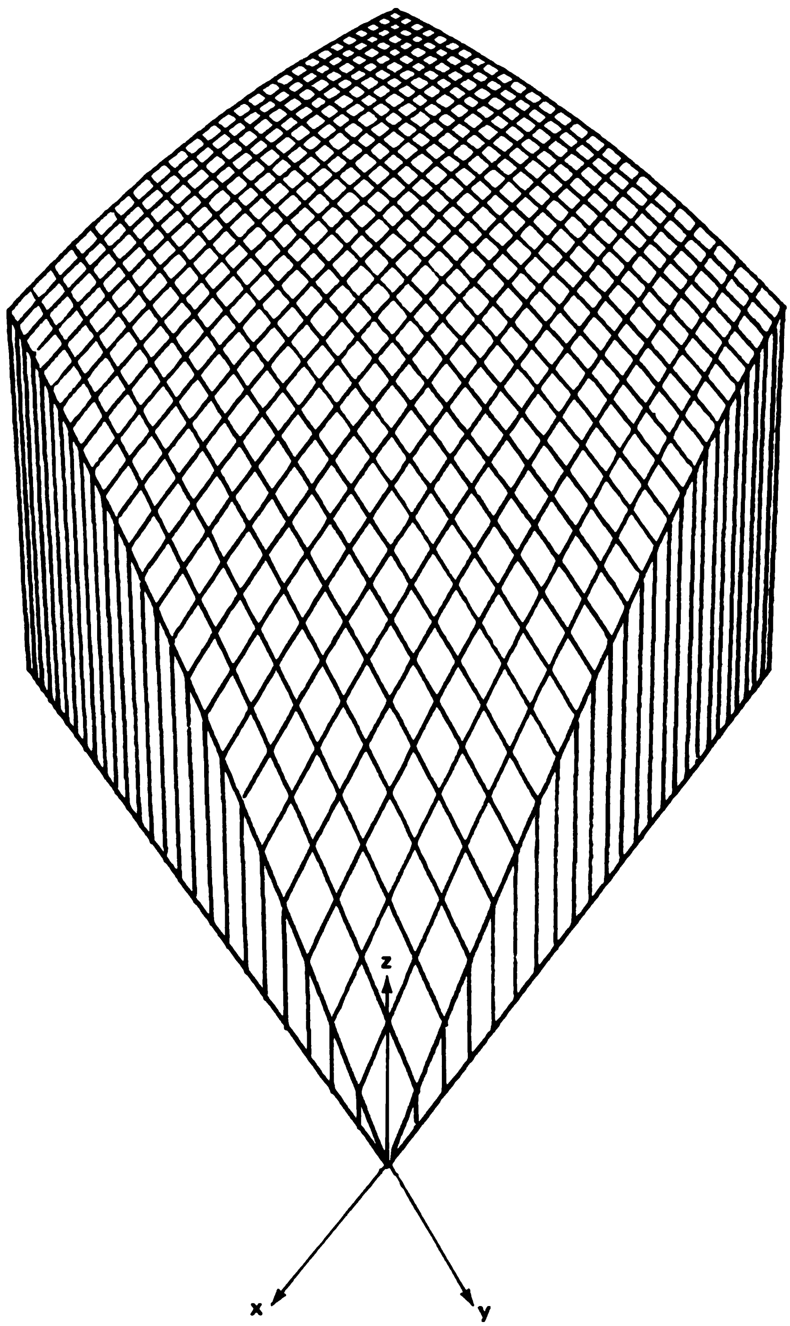


Figure 7.2.1.1 Graph of $z = \ln(xy)$ on $[1,2]^2$

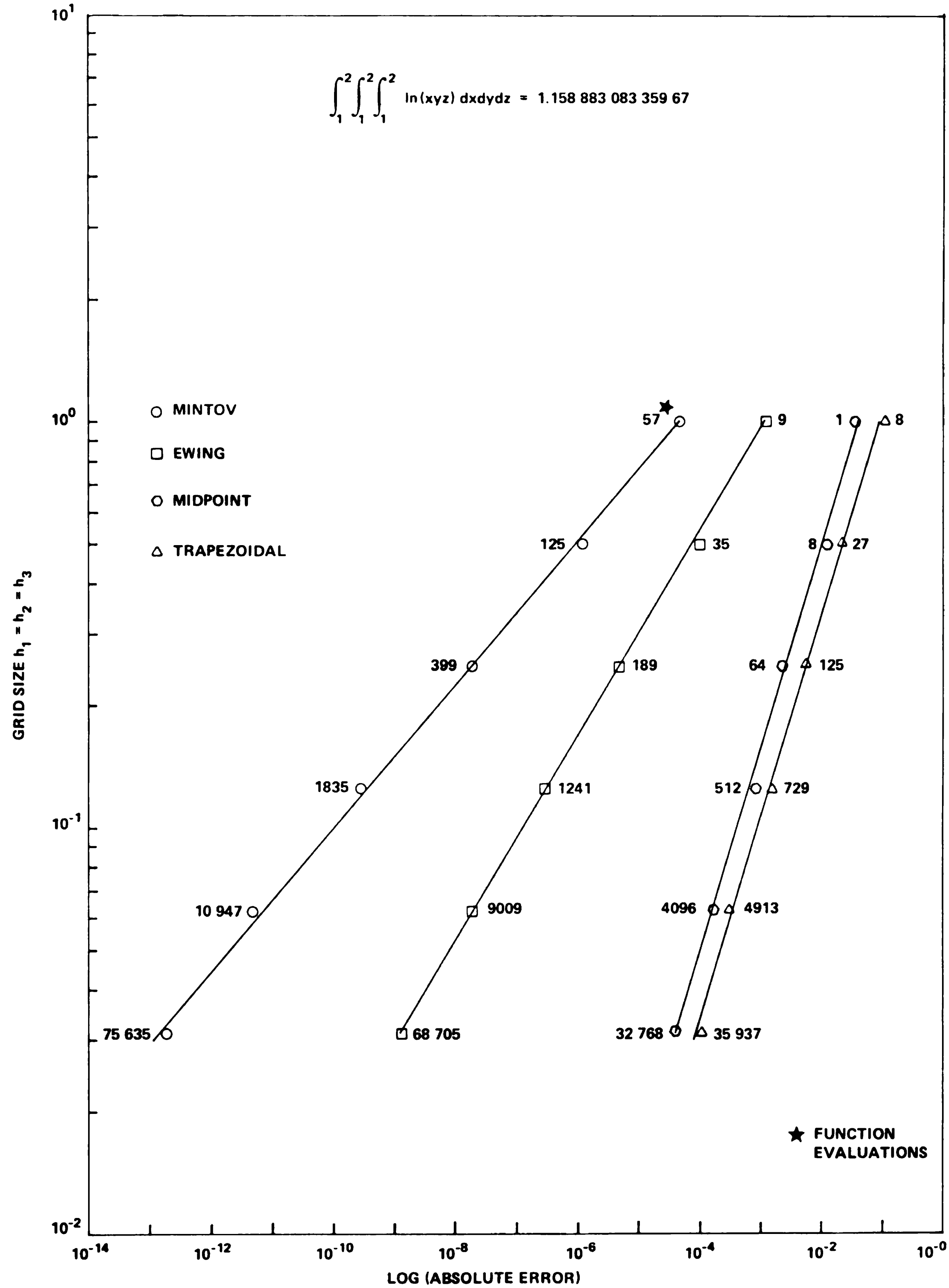


Figure 7.2.1.2 Error Curves in Approximating $\int_1^2\int_1^2\int_1^2 \ln(xyz)dxdydz$

The first-order partial derivatives of the function $f(x,y) = \ln(xyz)$ are much less costly to evaluate on a computer than is f. Moreover, the mixed second-order partials vanish everywhere. Thus it is of interest to apply MINTOV to this function. The results are presented in Table 7.2.1.1.

Table 7.2.1.1 $\int_1^2 \int_1^2 \int_1^2 \ln(xyz)dxdydz = 1.158\,883\,083\,359\,67$

Rule	$h_1 = h_2 = h_3 = 1$			$h_1 = h_2 = h_3 = 1/10$			Order
	nfe	Time (sec)	Error	nfe	Time (sec)	Error	
Trapezoidal	8	.002	1.19-1	1331	.457	1.25-3	1
Midpoint	1	.000	-5.75-2	1000	.361	-6.24-4	1
Ewing	9	.003	1.38-3	2331	.818	1.82-7	3
MINTOV	57	.009	-6.41-5	3189	.933	-1.14-10	5

For $h_1 = h_2 = h_3 = 1/10$, the MINTOV approximation is better than Ewing's result by 3 orders of magnitude. This confirms the theoretical result that the addition of partial derivative correction terms can greatly enhance a numerical integration formula.

7.2.2 MINTOV vs. JPL's MQUAD

Bunton, Diethelm, and Haigler [8] give the following example:

$$\int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \cos(x)\cos(y)\cos(z)\,dxdydz = 8.0. \tag{7.2.2.1}$$

The results of the DC-MQUAD algorithm using $n_1 = n_2 = n_3 = 2, 3, 5, 8, \cdots$, (cf. the Fibonnaci sequence) and JPL's routine MQUAD are presented in Table 7.2.2.1. Again, our method based on the 3-dimensional MINTOV formula (7.2.1) is superior to MQUAD.

Table 7.2.2.1 MINTOV vs. MQUAD for the Integral $\int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \cos(x)\cos(y)\cos(z)dxdydz = 8.$
Relative Errors Requested $= 10^{-a},\ a = 1(1)10.$

Relative Error Requested	MINTOV (DC-MQUAD Algorithm)			MQUAD (JPL Routine)		
	nfe	Time (sec)	Relative Error	nfe	Time (sec)	Relative Error
10^{-1}	360	.198	-1.11-3	2 197	1.634	8.74-5
10^{-2}	989	.546	-5.07-5	2 197	1.635	8.74-5
10^{-3}	2 824	1.529	-3.00-6	2 197	1.627	8.74-5
10^{-4}	2 824	1.529	-3.00-6	24 389	17.641	4.13-6
10^{-5}	9 109	4.971	-1.63-7	35 937	25.693	9.70-8
10^{-6}	32 186	17.558	-9.14-9	117 649	82.090	1.63-9
10^{-7}	122 135	66.611	-5.06-10	614 125	421.889	2.59-11
10^{-8}	122 135	66.611	-5.06-10	4 173 281	2 844.152	4.07-13
10^{-9}	483 614	264.343	-2.69-11	4 173 281	2 844.114	4.07-13
10^{-10}	1 967 263	1 076.794	1.55-11	31 855 013	21 647.323	8.40-15

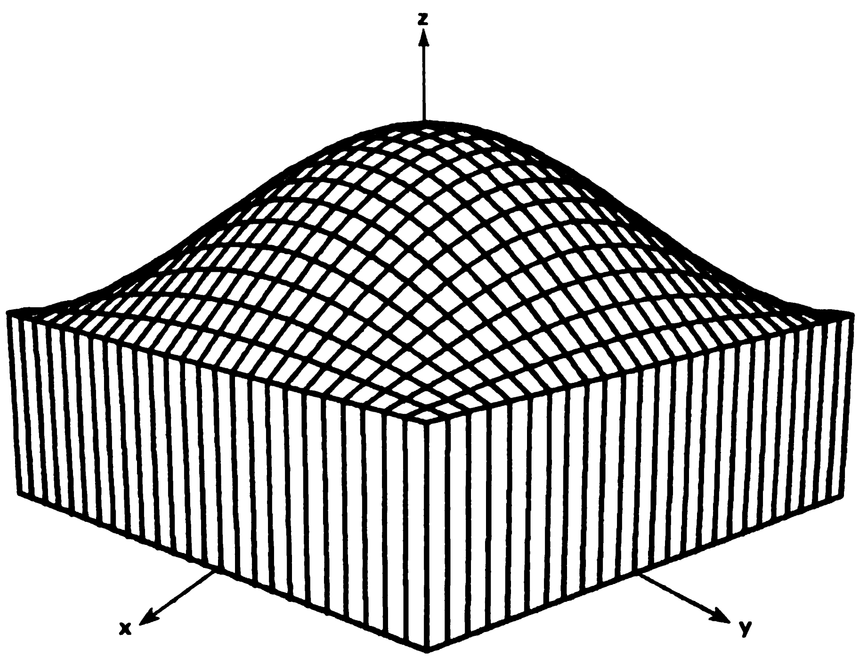


Figure 7.2.2.1 Graph of $z = \cos(x)\cos(y)$ on $[-\pi/2, \pi/2]^2$

7.2.3 AN EXAMPLE ILLUSTRATING THE PERSISTENCE OF FORM

Consider the integral

$$\int_0^{\pi/2}\int_0^{\pi/2}\int_0^{\pi/2} \frac{1+\sqrt{x^2+y^2+z^2}}{xyz} \sin(x)\sin(y)\sin(z)e^{-\sqrt{x^2+y^2+z^2}}\,dxdydz \tag{7.2.3.1}$$

$$= 1.531\,670\,226\,93.$$

If we let $w^2 = x^2 + y^2 + z^2$ then the first-order partial with respect to x is

$$f_x(x,y,z) = \left[(1+w)\cos(x) - (1+w+x^2)\frac{\sin(x)}{x}\right]\frac{\sin(y)\sin(z)e^{-w}}{xyz} \tag{7.2.3.2}$$

and the mixed second-order partial with respect to x and y is

$$\begin{aligned} f_{xy}(x,y,z) = \Bigg[&(1+w)\cos(x)\cos(y) + \frac{w+w^2+w(x^2+y^2)+x^2y^2}{wxy}\sin(x)\sin(y) \\ &- \frac{1+w+x^2}{x}\sin(x)\cos(y) - \frac{1+w+y^2}{y}\cos(x)\sin(y)\Bigg]\frac{\sin(z)e^{-w}}{xyz}. \end{aligned} \tag{7.2.3.3}$$

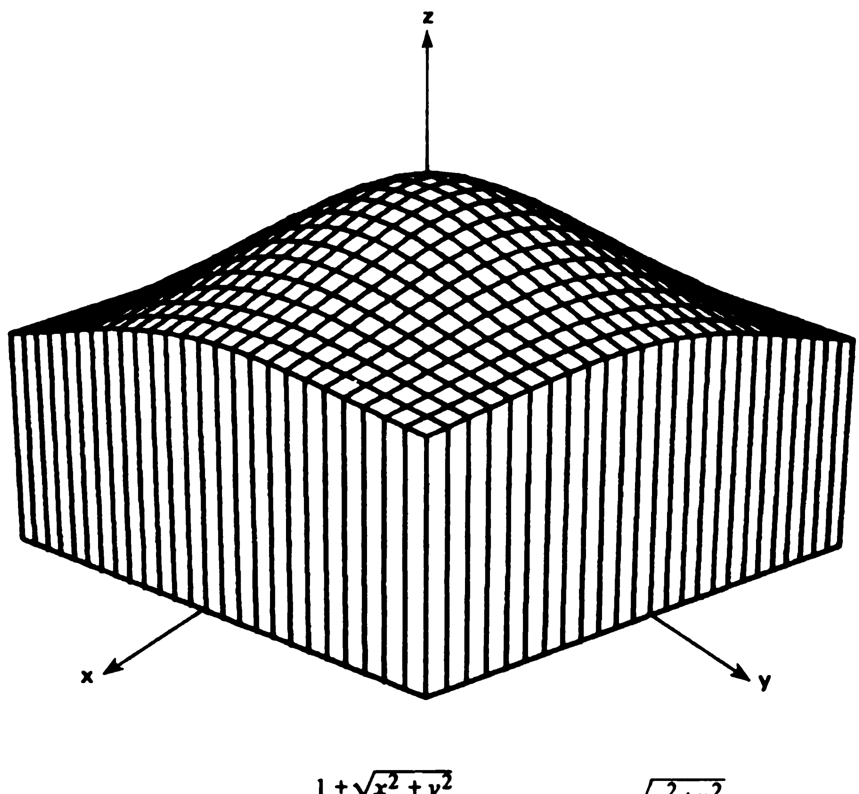


Figure 7.2.3.1 Graph of $z = \dfrac{1+\sqrt{x^2+y^2}}{xy}\sin(x)\sin(y)e^{-\sqrt{x^2+y^2}}$ on $[-\pi/2,\pi/2]^2$

The results of applying MINTOV with various grid sizes are presented in Table 7.2.3.1.

Table 7.2.3.1 $\int_0^{\pi/2}\int_0^{\pi/2}\int_0^{\pi/2} \frac{1+w}{xyz} \sin(x)\sin(y)\sin(z)\, e^{-w} dx\,dy\,dz = 1.531\,670\,226\,93$,

$w^2 = x^2 + y^2 + z^2$

$n_1=n_2=n_3$	Ewing			MINTOV		
	nfe	Time (sec)	Error	nfe	Time (sec)	Error
1	9	.007	-1.54-2	57	.048	-5.30-3
2	35	.031	-1.04-3	125	.111	-8.75-5
4	189	.174	-6.59-5	399	.364	-1.36-6
8	1 241	1.159	-4.13-6	1 835	1.712	-2.13-8
16	9 009	8.486	-2.58-7	10 947	10.314	-3.66-10
32	68 705	64.978	-1.62-8	75 635	71.579	-3.76-11
64	536 769	509.407	-1.03-9	562 899	534.424	-2.00-11

This example illustrates the persistence of form concept, namely, the cost of evaluating a derivative is approximately the same as the cost of evaluating the function.

In Table 7.2.3.1 for a given mesh size, the difference between the number of function evaluations required by MINTOV and Ewing is the number of partial derivative evaluations required by MINTOV. For example, for $n_1 = n_2 = n_3 = 16$, MINTOV uses 1938 first- and second-order partial derivative evaluations (pde) and takes 1.841 seconds, or an average of 950 microseconds per partial derivative evaluation (us/pde). This is to be compared with the conventional Ewing's formula which uses 9009 fe in 8.438 seconds, or an average of 937 us/fe. MINTOV averages 939 microseconds per evaluation, whether function or partial derivative.

Thus throughout this study we have weighted a partial derivative evaluation the same as a function evaluation, and refer to either simply as a function evaluation.

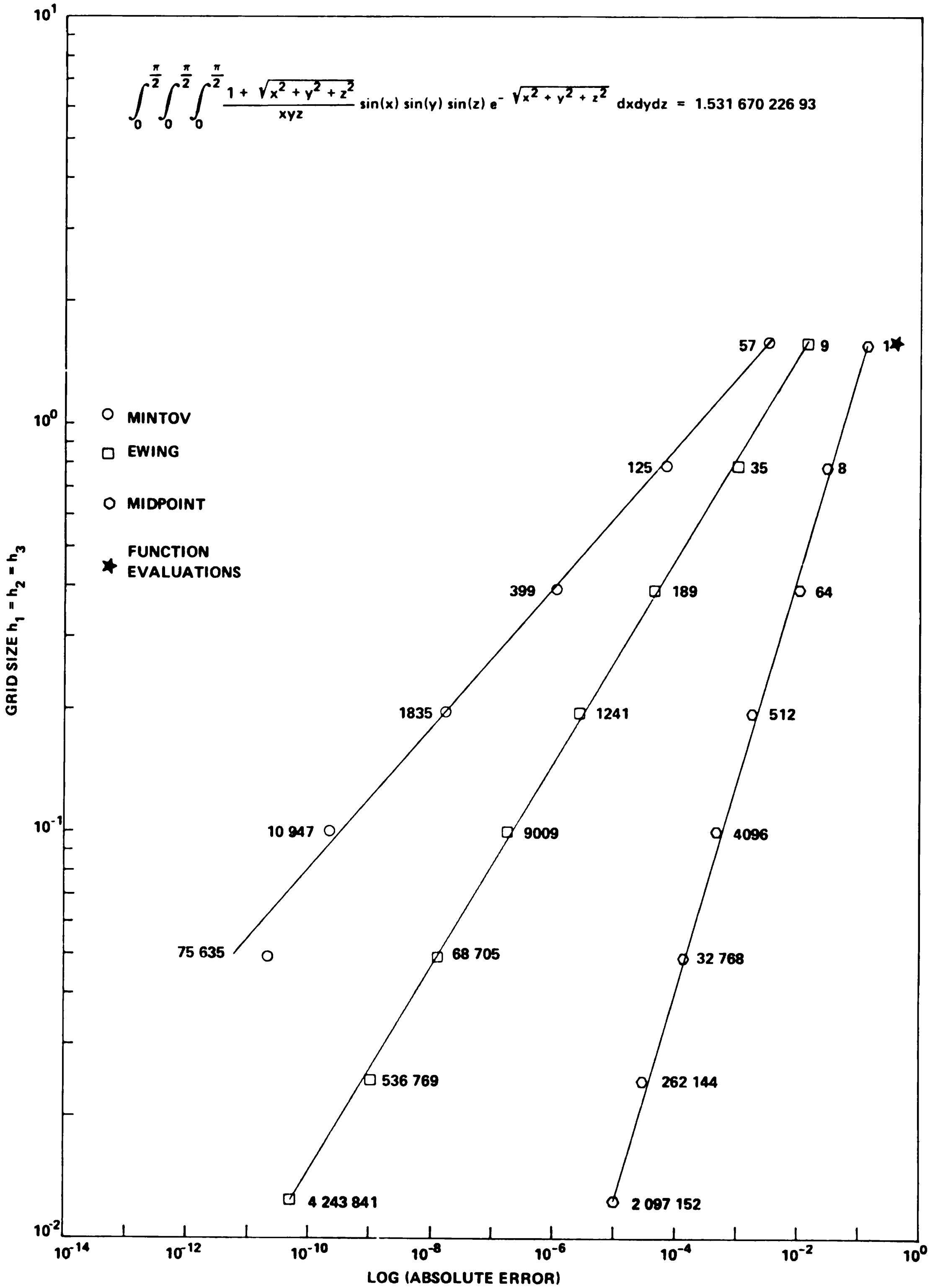


Figure 7.2.3.2 Error Curves

8. CONCLUSIONS AND RECOMMENDATIONS

We have studied the problem of enhancing the accuracy of conventional formulas for evaluating multiple integrals numerically over d-dimensional rectangles by the addition of partial derivative correction terms evaluated on the boundary of the domain of integration.

The formulas in Chapter 5 were based on the double Euler-Maclaurin Summation formula (5.2.1) and were found somewhat cumbersome to apply to practical situations because of the different weights for different nodes.

The formulas in Chapter 6, based on the finite Taylor Series expansion of the integrand, are much easier to apply in practice. We have constructed MINTOV (6.2.17), a fifth-order multi-dimensional integration formula which may be considered as the d-dimensional generalization of the 1-dimensional Lanczos quadrature formula (6.2.19) or of Ewing's cubature formula DØ5Ø3 given in Table 6.4.1.

For a single integral, the derivative correction terms are evaluated only at the end points of the interval of integration. The situation is somewhat more complicated in higher dimensions since, as the dimension increases, the boundary becomes increasingly more complex.

Of greater significance is the fact that in higher dimensions, most of the volume of a d-rectangle lies near the boundary. We have accounted for this by constructing multidimensional integration formulas with boundary partial derivative correction terms, the number of which increases as the dimension increases.

Indeed, as can be seen in (6.3.2), the d-dimensional MINTOV with n subdivisions requires n^d fe at the centroids of the subregions, $(n + 1)^d$ fe at lattice points, $2d(n + 1)^{d-1}$ first-order partial derivative evaluations at the lattice points of the $2d$ "faces" or $(d-1)$-dimensional hyperplanes, B, which bound the domain of integration, and $2d(d - 1)(n + 1)^{d-2}$ mixed second-order partial derivative evaluations at the lattice points of the 2^d "edges" or $(d - 2)$-dimensional hyperplanes which bound B.

In Chapter 6, 47 hitherto unpublished cubature formulas with boundary partial derivative correction terms were given. Computable bounds for the truncation errors were also given.

Three integration formulas, DF543S, XF543S, and OF843S (see Table 6.4.1) were discovered which require mixed second-order partial derivative correction terms evaluated only at the corners of the rectangular domain of integration. These formulas have the same error bound as Simpson's rule; however, they require far fewer function evaluations than Simpson's rule. Of the three, DF543S is the most efficient, requiring only half as many function evaluations as Simpson's rule.

OF543S has no interior nodes and yet it is not as efficient as DF543S which has one node interior to each cell. Thus, it is not always advisable to take as many points as possible on the boundary.

In cases where a third-order rule is considered adequate, DF543S should be preferred to Simpson's rule.

The fifth-order MINTOV was compared with JPL's routine MQUAD, and on the two test integrals considered, MINTOV required fewer function evaluations to achieve a prescribed relative error than did MQUAD.

The numerical results presented indicate that formula C5A or DH5G5S is an efficient and accurate composite fifth-order integration rule. For a sufficiently small grid size ($n = m = 4$ for a double integral, $n = m = 2$ for a triple integral, etc.) C5A requires fewer function evaluations than Simpson's rule.

Therefore, in situations where first- and mixed second-order partial derivatives are easily calculated, we have shown that the use of nodes satisfying the inclusion property coupled with the use of derivative correction terms exhibiting the equal weight-alternate sign property can improve the accuracy and efficiency of integration formulas. That is, whenever the first- and mixed second-order partial derivatives are easily computed, the formulas of Chapter 6 are to be preferred to conventional composite integration rules of comparable degrees.

Finally, future investigations should include the addition of weight functions, more general domains of integration, and the use of "difference correction terms."

LIST OF REFERENCES

GENERAL REFERENCES

Abramowitz, Milton
On the practical evaluation of integrals. J. Soc. Indust. Appl. Math 2 (1954) 20-35.

Abramowitz, Milton and Stegun, Irene A.
Handbook of Mathematical Functions. National Bureau of Standards. Applied Math. Series. V.55 (1964)

Aitken, A.C. and Frewin, G.L.
The Numerical Evaluation of Double Integrals. Proc. Edinburgh Math. Soc. 42 (1923) 2-13.

Anders, Edward B.
An Extension of Romberg Integration Procedures to N-Variables. J. ACM 13 (1966) 505-510.

Bailey, Carl B., Jones, Randall E.
Usage and Argument Monitoring of Mathematical Library Routines. ACM Trans. on Math. Software. 1 (1975) 196-209.

Baker, Christopher T.H. and Hodgson, Graham S.
Asymptotic Expansions for Integration Formulas in One or More Dimensions. SIAM J. Numer. Anal. 8 (1971) 473-480.

Barnes, E.W.
The Generalisation of the Maclaurin Sum Formula, and the Range of its Applicability. Quart. J. of Pure and Appl. Math. 35 (1904) 175-188.

Barrett, W.
On the Convergence of Cote's Quadrature Formulae. J. London Math. Soc. 39 (1964) 296-302.

Baten, William D.
A Remainder for the Euler-Maclaurin Summation Formula in Two Independent Variables. Amer. J. Math. 54 (1932) 265-275.

Bierens deHaan, David
Supplément aux Tables D'Intégrales Définies. Amsterdam: G.G. Van Der Post (1864).

Camp, C.C.
Note on Numerical Evaluation of Double Series. Ann. Math. Stat. 8 (1937) 72-75.

Chakravarti, P.C.
Integrals and Sums. Some New Formulae for their Numerical Evaluation. London: The Anthlone Press (1970).

Cody, W.J.
The Construction of Numerical Subroutine Libraries. SIAM Rev. 16 (1974) 36-46.

Cranley, R. and Patterson, T. N. L.
The Evaluation of Multidimensional Integrals. Comp. J. 11 (1968-69) 102-110.

Davis, Philip J. and Rabinowitz, Philip
Methods of Numerical Integration. New York: Academic Press (1975).

Frame, J.S.
Numerical Integration. Amer. Math. Monthly 50 (1943) 244-250.

Frank, Irving
An Application of the Euler-Maclaurin Sum Formula to Operational Mathematics. Quart. Appl. Math. 20 (1962) 89-91.

Gauss, C.F.
Methodus Nova Integralium Valores per Approximationem Inveniendi. Carl Friedrich Gauss Werke. Göttingen: Königlichen Gesellschaft der Wissenschaften 3 (1866) 163-196.

Ghizzetti, A., and Ossicini, A.
Quadrature Formulae. New York: Academic Press (1970).

Gibb, David
Interpolation and Numerical Integration. London: G. Bell & Sons, Ltd. (1915).

Gould, H.W. and Squire, William
Maclaurin's Second Formula and Its Generalization. Amer. Math. Monthly 70 (1963) 44-52.

Gradshteyn, I.S. and Ryzhik, I.M.
Tables of Integrals, Series, and Products. (Trans. from 4th Russian ed. by Alan Jeffrey). New York: Academic Press (1965).

Grant, J.A.
Derivation of Correction Terms for General Quadrature Formulae. Proc. Cambridge Phil. Soc. 66 (1969) 571-586.

Guenther, R.B. and Roetman, E.L.
Newton-Cotes Formulae in n-Dimensions. Numer. Math. 14 (1970) 330-345.

Haber, Seymour
Numerical Evaluation of Multiple Integrals. SIAM Rev. 12 (1970) 481-526.

Hammer, Preston C. and Wicke, Howard H.
Quadrature Formulas Involving Derivatives of the Integrand. Math. Comp. 14 (1960) 3-7.

Hamming, R.W. and Pinkham, R.S.
A Class of Integration Formulas. J. ACM 13 (1966) 430-438.

Håvie, T.
Derivation of Explicit Expressions for the Error Terms in the Ordinary and the Modified Romberg Algorithms. BIT 9 (1969) 18-29.

Håvie, T.
Some Algorithms for Numerical Quadrature Using the Derivatives of the Integrand in the Integration Interval. BIT 10 (1970) 277-294.

Hildebrand, F.B.
Introduction to Numerical Analysis. New York: McGraw-Hill Book Company. 2nd Ed., (1974).

Hillstrom, K.E.
Comparison of Several Adaptive Newton-Cotes Quadrature Routines in Evaluating Definite Integrals with Peaked Integrands. ANL-7511. Argonne Natl. Lab. Argonne, Il. (1968).

Hummel, P.M. and Seebeck, Jr., C.L.
A Generalization of Taylor's Expansion. Amer. Math. Monthly 56 (1949) 243-246.

Irwin, J.O.
On Quadrature and Cubature or On Methods of Determining Approximately Single and Double Integrals. London: Tracts for Computers. No. 10. Cambridge: Cambridge Univ. Press. (1923).

Isaacson, E. and Keller, H.B.
Analysis of Numerical Methods. New York: John Wiley & Sons, Inc. (1966).

Johnson, W. Woolsey
On Cotesian Numbers: Their History, Computation and Values to n=20. Quart. J. Pure Appl. Math. 46 (1915) 52-65.

Kahaner, David K.
Los Alamos Workshop on Quadrature Algorithms. SIGNUM Newsletter 11 (1976) 4-26.

Knuth, Donald E. and Buckholtz, Thomas J.
Computation of Tangent, Euler, and Bernoulli Numbers. Math. Comp. 21 (1967) 663-688.

Krylov, V.I. and Pal'tsev, A.A.
Tables for Numerical Integration of Functions with Logarithmic and Power Singularities. (Trans. from 1st Russian ed., 1967, by the Israel Program for Scientific Translations Staff). Jerusalem: Keter Press (1971).

Krylov, V.I. and Šulgina, L.T.
Handbook of Numerical Integration. (In Russian). Moscow: Izdat. Nauka. (1966).

Lambert, J.D. and Mitchell, A.R.
The Use of Higher Derivatives in Quadrature Formulae. Comp. J. 5 (1962-63) 322-327.

Lambert, John D. and Mitchell, Andrew R.
Repeated Quadratures Using Derivatives of the Integrand. Z. Angew. Math. Phys. 15 (1964) 84-90.

Lehmer, D.H.
An Extension of the Table of Bernoulli Numbers. Duke Math. J. 2 (1936) 460-464.

Lipow, Peter R. and Stenger, Frank
How Slowly Can Quadrature Formulas Converge? Math. Comp. 26 (1972) 917-922.

Lyness, J.N. and McHugh, B.J.J.
Integration Over Multidimensional Hypercubes. I. A Progressive Procedure. Comp. J. 6 (1963-64) 264-270.

Lyness, J.N. and Ninham, B.W.
Numerical Quadrature and Asymptotic Expansions. Math. Comp. 21 (1967) 162-178.

McNamee, John
Error-Bounds for the Evaluation of Integrals by the Euler-Maclaurin Formula and by Gauss-Type Formulae. Math. Comp. 18 (1964) 368-381.

Maxwell, J. Clerk
On Approximate Multiple Integration between Limits of Summation. Proc. Cambridge Phil. Soc. 3 (1877) 39-47.

Miller, J.C.P.
Quadrature in Terms of Equally-Spaced Function Values. U.S. Army Math. Research Center, Madison, Wisc. Rep. 167, July, 1960, 1-91.

Munro, W.D.
Note on the Euler-Maclaurin Formula. Amer. Math. Monthly 65 (1958) 201-203.

Mysovskih, I.P.
Lectures on Numerical Methods. Groningen, The Netherlands; Wolters-Noordhopf Publishing (1969).

Nikol'skii, S.M.
Quadrature Formulae. (Trans. from the 1st Russian ed., 1958) Delhi: Hindustan Publishing Corp. (1964).

Northam, Jack I.
Certain Summation and Cubature Formulas. East Lansing: Michigan State University. Master's thesis (1939).

Ohm, M.
Etwas Über die Bernoullischen Zahlen. J. Reine Angew. Math. 20 (1840) 11-12.

Patterson, T.N.L.
Integration Formulae Involving Derivatives. Math. Comp. 23 (1969) 411-412.

Philips, G.M.
Numerical Integration in Two and Three Dimensions. Comp. J. 10 (1967) 202-204.

Ralston, A.
A Family of Quadrature Formulas Which Achieve High Accuracy in Composite Rules. J. ACM 6 (1959) 384-394.

Rosenstock, Herbert B.
Euler-Maclaurin Formula in Three Dimensions. J. Math. and Phys. 43 (1964) 342-346.

Sack, R.A.
Newton-Cotes Type Quatrature Formulas with Terminal Corrections. Comp. J. 5 (1962-63) 230-237.

Sadowsky, Michael
A Formula For Approximate Computation of a Triple Integral. Amer. Math. Monthly 47 (1940) 539-543.

Saidel, Frank
Some Interpolation Formulas in Two Variables. East Lansing: Michigan State University. Masters thesis (1941).

Scarborough, J.B.
On the Relative Accuracy of Simpson's Rules and Weddle's Ruie. Amer. Math. Monthly 34 (1927) 135-139.

Scarborough, James B.
Numerical Mathematical Analysis. Baltimore: The Johns Hopkins Press. 5th ed. (1962).

Schoenberg, I.J. and Sharma, A.
The Interpolatory Background of the Euler-Maclaurin Quadrature Formula. Bull. AMS 77 (1971) 1034-1038.

Shampine, Lawrence F.
Quadrature Formulas Using Derivatives. Math. Comp. 19 (1965) 481-482.

Smith, Francis J.
Quadrature Methods Based on the Euler-Maclaurin Formula and on the Clenshaw-Curtis Method of Integration. Numer. Math. 7 (1965) 406-411.

Smith, J.M.
Recent Developments in Numerical Integration. J. Dynamic Systems, Measurement, and Control. March (1974) 61-70.

Squire, William
Some Applications of Quadrature by Differentiation. J. Soc. Indust. Appl. Math. 9 (1961) 94-108.

Steffensen, J.F.
Interpolation. New York: Chelsea Publ. Co., 2nd ed. (1950).

Ström, Torsten
Strict Error Bounds in Romberg Quadrature. BIT 7 (1967) 314-321.

Stroud, A.H.
Quadrature Methods for Functions of More Than One Variable. Ann. NY Acad. Sci. 86 (1960) 776-791.

Stroud, A.H.
A Bibliography on Approximate Integration. Math. Comp. 15 (1961) 52-80.

Stroud, A.H.
Numerical Quadrature and Solution of Ordinary Differential Equations. New York: Springer-Verlag (1974).

Stroud, A.H. and Secrest, D.
Gaussian Quadrature Formulas. Englewood Cliffs: Prentice-Hall, Inc. (1966).

Strubble, George
Tables for Use in Quadrature Formulas Involving Derivatives of the Integrand. Math. Comp. 14 (1960) 8-12.

Takeyama, Hisao
Expressions for Interpolation and Numerical Integration of High Accuracy. Tôhoku Univ. Technology Reports. 23 (1958) 47-70.

Thacher, Jr., Henry C.
An Efficient Composite Formula for Multidimensional Quadrature. Comm. ACM 7 (1964) 23-25.

Tyler, G.W.
Numerical Integration of Functions of Several Variables. Canadian J. Math. 5 (1953) 393-412.

Uspensky, J.V.
On an Expansion of the Remainder in the Gaussian Quadrature Formula. Bull. AMS 40 (1934) 871-876.

Weddle, Thomas
On a New and Simple Rule for Approximating to the Area of a Figure by Means of Seven Equidistant Ordinates. Cambridge Math. J. 9 (1854) 79-80.

BIBLIOGRAPHY

1 Adams, J.C.
Table of the values of the first sixty-two numbers of Bernoulli. J. Reine Angew. Math. 85 (1878) 269-272.

2 Ahlin, A.C.
On Error Bounds for Gaussian Cubature. SIAM Rev. 4 (1962) 25-39.

3 Albrecht, J., and Collatz, L.
Zur Numerischen Auswertung Mehrdimensionaler Integrale, Z. Angew. Math. Mech. 38 (1958) 1-15.

4 Barnes, E.W.
The Maclaurin Sum-Formula. Proc. London Math. Soc. 3 (1905) 253-272.

5 Bauer, F.L., Rutishauser, H., and Stiefel, E.
New Aspects in Numerical Quadrature. Proc. Symp. Appl. Math. Providence: Amer. Math. Soc. 15 (1963) 199-218.

6 Becker, George F.
Some New Mechanical Quadratures. Philos. Mag. 22 (1911) 342-353.

7 Bickley, W.G.
Finite Difference Formulae for the Square Lattice. Quart. J. Mech. Appl. Math. 1 (1948) 35-42.

8 Bunton, Wiley R., Diethelm, Michael, and Haigler, Karen
Romberg Quadrature Subroutines for Single and Multiple Integrals. Jet Propulsion Lab., Pasadena, Calif. TM-314-221. July 1, 1969, 1-50.

9 Bunton, Wiley R., and Diethelm, Michael
Modifications to the JPL Romberg Subroutines. Jet Propulsion Lab., Pasadena, Calif. TM-314-247. September 1, 1970, 1-9.

10 Bunton, Wiley R., Diethelm, Michael, and Winje, Gilbert L.
Modified Romberg Quatrature: A Subroutine to Support General Scientific Computing. Jet Propulsion Lab., Pasadena, Calif. TM-314-258. April 1, 1970, 1-35.

11 Burnside, W.
An Approximate Quadrature Formula. Messenger of Math. 37 (1908) 166-167.

12 Caselleto, J., Pickett, M., and Rice, J.
A Comparison of Some Numerical Integration Programs. SIGNUM Newsletter. 4 (1969) 30-40.

13 Davis, Philip J., and Rabinowitz, Philip
Methods of Numerical Integration. New York: Academic Press (1975).

14 DeDoncker, Elise, and Piessens, Robert
A Bibliography on Automatic Integration. J. Comput. and Appl. Math. (to appear).

15 Euler, Leonhard
Methodus Generalis Summandi Progressiones. Commentarii Acad. Sci. Imp. Petropolitanae. Vol. 6 (1732-33, published 1738) St. Petersburg.

16 Ewing, G.M.
On Approximate Cubature. Amer. Math. Monthly. 48 (1941) 134-136.

17 Forsythe, George E., and Moler, Cleve B.
Computer Solution of Linear Algebraic Systems. Englewood Cliffs: Prentice-Hall (1967).

18 Frame, J. Sutherland
Numerical Integration and the Euler-Maclaurin Summation Formula. East Lansing: Michigan State University (to appear).

19 Fritsch, F.N.
A Bibliography on Approximate Multidimensional Integration 1960-1968. Lawrence Radiation Lab., Livermore, Calif. UCRL-50610. March 5, 1969, 1-20.

20 Good, I.J., and Gaskins, R.A.
The Centroid Method of Numerical Integration. Numer. Math. 16 (1971) 343-359.

21 Hammer, Preston C.
Numerical Evaluation of Multiple Integrals. On Numerical Approximation. Langer, R.E. (Ed.) (Proceedings of a symposium conducted by the U.S. Army Math. Research Center). Madison: The University of Wisconsin Press (1959), 99-115.

22 Hammer, Preston C., and Wymore, A. Wayne
Numerical Evaluation of Multiple Integrals I. MTAC 11 (1957) 59-67.

23 Ionescue, D.V.
Generalization of the Quadrature Formula of N. Obreschkoff for Double Integrals (In Romanian). Stud. Cerc. Mat. 17 (1965) 831-841.

24 Joyce, D.C.
Survey of Extrapolation Process in Numerical Analysis. SIAM Rev. 13 (1971) 435-490.

25 Kahaner, D.K.
Comparison of Numerical Quadrature Formulas. Mathematical Software. J. R. Rice (ed.). New York: Academic Press (1970) 229-259.

26 Knopp, K.
Theory and Application of Infinite Series. London: Blackie and Son (1951).

27 Krylov, V.I.
Approximate Calculation of Integrals. (Trans. from 1st Russian ed., 1959, by A. H. Stroud) New York: Macmillan Company (1962).

28 Lanczos, C.
Applied Analysis. Englewood Cliffs: Prentice-Hall (1956).

29 Lyness, J.N.
Symmetric Integration Rules for Hypercubes I. Error Coefficients. Math. Comp. 19 (1965) 260-276.

30 Lyness, J.N., and Kaganove, J.J.
A Technique for Comparing Automatic Quadrature Routines. Private communication (1975).

31 Lyness, J.N., and Kaganove, J.J.
Comments on the Nature of Automatic Quadrature Routines. ACM Trans. on Math. Software. 2 (1976) 65-81.

32 Lyness, J.N., and McHugh, B.J.J.
On the Remainder Term in the *N*-Dimensional Euler Maclaurin Expansion. Numer. Math. 15 (1970) 333-344.

33 Maclaurin, Colin
A Treatise on Fluxions. Edinburgh (1742), p. 672.

34 Meister, Bernd
On a Family of Cubature Formulae. Comp. J. 8 (1966) 368-371.

35 Miller, J.C.P.
Numerical Quadrature over a Rectangular Domain in Two or More Dimensions. I Quadrature over a Square using up to Sixteen Equally Spaced Points. Math. Comp. 14 (1960) 13-20.

36 Milne, W.E.
Numerical Calculus. Princeton: Princeton University Press (1949).

37 Mustard, D., Lyness, J.N., and Blatt, J.M.
Numerical Quadrature in *N* Dimensions. Comp. J. 6 (1963-64) 75-87.

38 Obreschkoff, N.
Neue Quadraturaturformeln. Abhandlungen der Preussischen Akademie der Wissenschaften. Berlin. 4 (1940) 1-20.

39 Oliver, F.W.J.
Asymptotics and Special Functions. New York: Academic Press (1974).

40 Oliver, J.
The Evaluation of Definite Integrals Using High-Order Formulae. Comp. J. 14 (1971) 301-306.

41 Price, J.F.
Examples and Notes on Multiple Integration. Boeing Scientific Research Lab., Seattle, Wash. Mathematical Note No. 285, D1-82-0231 (1963), 1-34.

42 Radon, Johann
Zur Mechanischen Kubatur. Monatsh. Math. 52 (1948) 286-300.

43 Richardson, L.F., and Gaunt, J.A.
The Deferred Approach to the Limit. Trans. Roy. Soc. London 226A (1927) 299-361.

44 Romberg, Werner
Vereinfachte Numerische Integration. Norske Vid. Selsk. Forh. Trondheim 28 (1955) 30-36.

45 Sheppard, W.F.
Some Quadrature-Formulae. Proc. London Math. Soc. 32 (1900) 258-277.

46 Simpson, T.
Mathematical Dissertations. London (1743).

47 Squire, William
Integration for Engineers and Scientists. New York: Amer. Elsevier Pub. Company (1970).

48 Squire, William
Numerical Evaluation of a Class of Singular Double Integrals by Symmetric Pairing. Intl. J. for Numer. Meth. in Engr. 10 (1976) 703-708.

49 Stroud, A.H.
Approximate Calculation of Multiple Integrals. Englewood Cliffs: Prentice-Hall (1971).

50 Tanimoto, B.
An Efficient Modification of Euler-Maclaurin's Formula. Trans. Japan Soc. Civil Engrs. 24 (1955) 1-5.

51 Tyler, George W.
The Experimental Evaluation of Definite Integrals. Blacksburg: Virginia Polytechnic Institute and State University. Ph.D. dissertation (1949).

52 Uspensky, J.V.
On the Expansion of the Remainder in the Newton-Cotes Formula. Trans. AMS 37 (1935) 381-396.