## Numerical Quadrature Over a Rectangular Domain in Two or More Dimensions

Part 1. Quadrature over a Square, Using up to Sixteen Equally Spaced Points

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1. Introduction. Except for a section of a paper by Bickley [1] which gives some of the results that follow, there seems to be very little in print concerning numerical quadrature over rectangular domains in two or more dimensions. This is perhaps because numerical evaluations can be readily made by using one-dimensional formulas on each variable in turn—such formulas as the Euler-Maclaurin formula, Gregory's formula, Simpson's rule, Newton's three-eighths rule, or Gauss's formulas, to name a few. This restriction to "products" of one-dimensional formulas limits the field unduly, and may lead to an excessively large amount of work. Thus, in n dimensions, use of Gauss's 3-point formula involves  $3^n$  points, whereas comparable accuracy may be obtained with about  $2n^2$  points.

In this first note we explore some of the simple possibilities corresponding to Simpson's rule and the three-eighths rule, applied to 9 or 16 points equally spaced over a square, the corner points being included.

2. Integration over a Square. We restrict the domain of integration to be a square; this covers any rectangular domain by change of scale. We take the center of the square as origin of coordinates, and in the first place take the side of the square to be 2h; and the integral as

(2.1) 
$$I = \int_{-h}^{h} \int_{-h}^{h} f(x, y) \, dx \, dy.$$

We assume that f(x, y) can be expanded as far as we need in a Taylor series in x and y. In other words, we suppose that f(x, y) can be represented adequately by a polynomial in x and y, with an error term which we shall suppose may be estimated by considering a few of the more significant neglected terms. We shall not give an accurate error analysis.

It is clear that polynomial terms involving an odd power of either variable will contribute nothing to the integral; we shall also group ordinates in sets such that the total contribution to their sum is zero for such terms involving an odd power of either variable. For example, the points (h, 0), (-h, 0), (0, h), (0, -h) form one such group. With this grouping we can then eliminate from consideration all terms of the Taylor expansion which do not involve an even power of both variables.

3. Method of Derivation. We seek approximate formulas of the form

(3.1) 
$$I = \int_{-h}^{h} \int_{-h}^{h} f(x, y) \, dx \, dy \doteq \sum A_{r,s}(rh, sh)$$

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in which  $A_{r,s} = A_{s,r} = A_{|r|,|s|}$ , and which will be exact for appropriate polynomial functions f(x, y) of sufficiently low degree.

Two approaches, not entirely distinct, may be used:

(i) We may give f(x, y) special forms and choose coefficients  $A_{r,s}$  to fit these exactly. Such forms are 1,  $x^2$  (or the equivalent symmetrical form  $x^2 + y^2$ ),  $x^4$ ,  $x^2y^2$ , etc

(ii) We may expand f(x, y) as a Taylor series and evaluate I both by means of the integral and by means of the sum, and equate coefficients.

We shall give an example of each approach, in order to bring out an interesting point concerning the proper choice of special forms.

4. Nine-point Formulas (i). Consider the nine points, grouped as indicated by the semi-colons: (0, 0); (h, 0), (-h, 0), (0, h), (0, -h); (h, h), (-h, h), (h, -h), (-h, -h); and the four special functions f(x, y) = 1,  $x^2$ ,  $x^4$ ,  $x^2y^2$  with values at the nine points as follows

(4.1)	1 1 1	1 1 1	1 1 1		1 1 1	0 0 0	1 1 1		1 1 1	0 0 0	1 1 1		1 0 1	0 0 0	1 0 1	
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The values of  $I/4h^2$  are

 $(4.2) 1, \frac{1}{3}, \frac{1}{5}, \frac{1}{9}.$ 

Hence, we wish to have

(4.3) 
$$\begin{cases} A_{0,0} + 4A_{1,0} + 4A_{1,1} = 1\\ 2A_{1,0} + 4A_{1,1} = \frac{1}{3}\\ 2A_{1,0} + 4A_{1,1} = \frac{1}{5}\\ 4A_{1,1} = \frac{1}{9} \end{cases}$$

We note at once that two of the equations are incompatible. Since we have 4 equations for 3 unknowns, we can still solve them if we discard the third (since the correct result for  $x^2$  must have precedence over the correct result for  $x^4$ ). We obtain

$$A_{0,0} = \frac{4}{9}$$
  $A_{1,0} = \frac{1}{9}$   $A_{1,1} = \frac{1}{36}$ 

which is precisely the Simpson's rule "product," see Bickley [1], eq. (22), with multipliers

(A) 
$$\begin{vmatrix} 1 & 4 & 1 \\ 4 & 16 & 4 \\ 1 & 4 & 1 \end{vmatrix} \div 36$$

to give  $I/4h^2$ . The main error term clearly concerns the coefficients of the terms in  $x^4$  and  $y^4$  and is

$$\frac{h^4}{180}\left(\frac{\partial^4 f}{\partial x^4}+\frac{\partial^4 f}{\partial y^4}\right)_{0,0}.$$

5. Nine-point Formulas (ii). We now consider the same problem by expanding and equating coefficients. We have, using  $f_{r,s}$  for f(rh, sh), and  $f_0$  simply for f(0, 0),

$$(5.1) \quad f(x, y) = f_0 + \frac{x^2}{2!} \frac{\partial^2 f_0}{\partial x^2} + \frac{y^2}{2!} \frac{\partial^2 f_0}{\partial y^2} + \frac{x^4}{4!} \frac{\partial^4 f_0}{\partial x^4} + \frac{6x^2 y^2}{4!} \frac{\partial^4 f_0}{\partial x^2 \partial y^2} + \frac{y^4}{4!} \frac{\partial^4 f_0}{\partial y^4} + \cdots$$

whence

(5.2) 
$$I = 4h^2 \left[ f_0 + \frac{h^2}{3!} \left( \frac{\partial^2 f_0}{\partial x^2} + \frac{\partial^2 f_0}{\partial y^2} \right) + \frac{h^4}{5!} \left( \frac{\partial^4 f_0}{\partial x^4} + \frac{10}{3} \frac{\partial^4 f_0}{\partial x^2 \partial y^2} + \frac{\partial^4 f_0}{\partial y^4} \right) + \cdots \right]$$

Following Bickley [1], we write this concisely in terms of

(5.3) 
$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \text{ and } \mathfrak{D}^4 \equiv \frac{\partial^4}{\partial x^2 \partial y^2}$$

Then, adding further terms for later use,

(5.4)  
$$I/4h^{2} = f_{0} + \frac{h^{2}}{3!}\nabla^{2}f_{0} + \frac{h^{2}}{5!}(\nabla^{4}f_{0} + \frac{4}{3}\mathfrak{D}^{4}f_{0}) + \frac{h^{6}}{7!}(\nabla^{6}f_{0} + 4\mathfrak{D}^{4}\nabla^{2}f_{0}) + \frac{h^{8}}{9!}(\nabla^{8}f_{0} + 8\mathfrak{D}^{4}\nabla^{4}f_{0} + \frac{16}{5}\mathfrak{D}^{8}f_{0}) + \cdots$$

•

We have likewise

$$(5.5) \begin{cases} f_{0,0} = f_{0} \\ f_{1,0} + f_{0,1} + f_{-1,0} + f_{0,-1} = 4f_{0} + \frac{2}{2!}h^{2}\nabla^{2}f_{0} + \frac{2}{4!}h^{4}(\nabla^{4}f_{0} - 2\mathfrak{D}^{4}f_{0}) \\ + \frac{2}{6!}h^{6}(\nabla^{6}f_{0} - 3\mathfrak{D}^{4}\nabla^{2}f_{0}) + \frac{2}{8!}h^{8}(\nabla^{8}f_{0} - 4\mathfrak{D}^{4}\nabla^{4}f_{0} + 2\mathfrak{D}^{8}f_{0}) + \cdots \\ f_{1,1} + f_{-1,1} + f_{1,-1} + f_{-1,-1} = 4f_{0} + \frac{4}{2!}h^{2}\nabla^{2}f_{0} + \frac{4}{4!}h^{4}(\nabla^{4}f_{0} + 4\mathfrak{D}^{4}f_{0}) \\ + \frac{4}{6!}h^{6}(\nabla^{6}f_{0} + 12\mathfrak{D}^{4}\nabla^{2}f_{0}) + \frac{4}{8!}h^{8}(\nabla^{8}f_{0} + 24\mathfrak{D}^{4}\nabla^{4}f_{0} + 16\mathfrak{D}^{8}f_{0}) + \cdots \end{cases}$$

From these relations we obtain, for terms to  $h^4$  in  $I/4h^2$ 

(5.6) 
$$\begin{cases} A_{0,0} + 4A_{1,0} + 4A_{1,1} = 1\\ 2A_{1,0} + 4A_{1,1} = \frac{1}{3}\\ 2A_{1,0} + 4A_{1,1} = \frac{1}{5}\\ -4A_{1,0} + 16A_{1,1} = \frac{4}{15} \end{cases}$$

The first three equations are as in (4.3), and the second and third remain incompatible. Neglecting the third we can solve to give (see Bickley [1], eq. (20)) the multipliers for  $I/4h^2$ ;

The difference in the fourth equation between (4.3) and (5.6) leads to different formulas. The cause is reflected in the error term. In the second case we have ignored a term in  $\nabla^4 f_0$  and removed the remaining term in  $D^4 f_0$ ; in 4 we have ignored a term in

$$\left(\frac{\partial^4 f_0}{\partial x^4} + \frac{\partial^4 f_0}{\partial y^4}\right)$$

and removed the remaining term in  $\mathfrak{D}^4 f_0$ . The error term in the product-Simpson formula can be expressed alternatively in the form

$$\frac{h^4}{180} \left( \nabla^4 f_0 - 2 \mathfrak{D}^4 f_0 \right).$$

It is perhaps a moot point which formula will give better results, unless it is known that f(x, y) is exactly, or almost a harmonic function. It is perhaps worth noting that for the method of 4 to yield the formula (B) it is necessary only to take a harmonic function instead of  $x^2y^2$  in deriving the last equation. For example,  $f(x, y) = x^4 - 6x^2y^2 + y^4$  gives values

(5.7) 
$$\begin{array}{c|c} -4 & 1 & -4 \\ 1 & 0 & 1 \\ -4 & 1 & -4 \end{array} \quad \text{and } I/4h^2 = -\frac{4}{15}h^4$$

and the fourth equation

$$(5.8) -4A_{1,0} + 16A_{1,1} = \frac{4}{15}$$

6. Five-point and Other Formulas. The impossibility of removing all of the  $h^4$  terms in the error in  $I/4h^2$  by using 9 points, suggests the possibility of using fewer points, in fact five or eight, while still retaining an error of order  $h^4$ . There are three possibilities, using the first two equations only of (4.3) or (5.6).

(i) Take  $A_{0,0} = 0$ ; this yields multipliers

(C) 
$$\begin{vmatrix} -1 & 4 & -1 \\ 4 & 0 & 4 \\ -1 & 4 & -1 \end{vmatrix} \div 12$$
 with main error  $\frac{1}{180}h^4(\nabla^4 f_0 - 22\mathfrak{D}^4 f_0)$ .

(ii) Take 
$$A_{1,1} = 0$$
, giving

(D) 
$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 0 \end{bmatrix} \div 6$$

with main error 
$$\frac{1}{180}h^4(\nabla^4 f_0 - 7\mathfrak{D}^4 f_0)$$
.

(iii) Take  $A_{1,0} = 0$ , giving the "diagonal Simpson's rule"

(E) 
$$\begin{vmatrix} 1 & 0 & 1 \\ 0 & 8 & 0 \\ 1 & 0 & 1 \end{vmatrix} \div 12$$

with main error  $\frac{1}{180}h^4(\nabla^4 f_0 + 8\mathfrak{D}^4 f_0)$ .

The first of these has little to commend it, with its large  $\mathfrak{D}^4 f_0$  error term, and its negative multipliers. The other two (see Bickley [1], eqs. (23, 24)) are reasonably good. Over large areas, with many contiguous squares of area  $4h^2$ , they average respectively 3 and 2 points per square. With a square of side 6h, for example, they give

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	8	0 4 0	8 0 8	0 4 0	0 8	$0 \\ 2$	
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The first of these has interior points with multipliers 2 (or zero) only. We note also that combination in proportions  $\frac{8}{15}$ :  $\frac{7}{15}$  gives precisely the formula (B). One further formula is obtained by combining (D) and (E) in equal proportions:

(G) 
$$\begin{vmatrix} 1 & 2 & 1 \\ 2 & 12 & 2 \\ 1 & 2 & 1 \end{vmatrix} \div 24$$
with main error  $\frac{1}{1 \ge 0} h^4 (\nabla^4 f_0 + \frac{1}{2} \mathfrak{D}^4 f_0)$ 

and with simple multipliers and a good error term.

7. 16-point Formulas. These follow exactly the pattern for nine-point formulas; we merely quote results.

The method of 4, with the same special functions, and with similar neglect of the incompatible third equation gives for  $I/9h^2$ , where

$$I = \int_{-3h/2}^{3h/2} \int_{-3h/2}^{3h/2} f(x, y) \, dx, \, dy,$$

 $\div 64$ 

the multipliers

with main error term 
$$\frac{1}{50}h^3(\nabla^4 f_0 - 2\mathfrak{D}^4 f_0)$$

The formula corresponding to (B) of 5 is

with main error term  $\frac{1}{80}h^4\nabla^4 f_0$ .

8. Twelve-point Formulas and Others. As in 6 we can use the first two equations after setting one of the coefficients  $A_{1,1}$ ,  $A_{1,3}$ , or  $A_{3,3}$  equal to zero. This yields

twelve-point formulas (i) with  $A_{1,1} = 0$ :  $\begin{vmatrix} -2 & 3 & 3 & -2 \\ 3 & 0 & 0 & 3 \\ 3 & 0 & 0 & 3 \\ -2 & 3 & 3 & -2 \end{vmatrix} \div 16$  with main error term  $\frac{1}{80}h^4(\nabla^4 f_0 - 47\mathfrak{D}^4 f_0)$ (C') (ii) with  $A_{3,3} = 0$ : (D') (iii) The "diagonal three-eighths rule", with  $A_{1,3} = 0$ : (E')

Also, as in 6, we may combine the last two in the ratio  $\frac{1}{3}$ : $\frac{2}{3}$ , to give

(G') 
$$\begin{vmatrix} 1 & 2 & 2 & 1 \\ 2 & 7 & 7 & 2 \\ 2 & 7 & 7 & 2 \\ 1 & 2 & 2 & 1 \\ 1 & 2 & 2 & 1 \end{vmatrix} \div 48$$
 with main error term  $\frac{1}{30}h^4(\nabla^4 f_0 - \frac{1}{3}\mathfrak{D}^4 f_0)$ .

Finally, we write out multipliers over a square of side 6h for the 12-point formulas (ii) and (iii) above (which average respectively 8 and 5 points per square of side 3h)

(F')	1 1 0 1 1	2 2 2 2 2	2 2 2 2	2 2 0 2 2	2 2 2 2 2 2	2 2 2 2 2 2	1 1 0 1 1	÷ 16	0 0 1 0 0	3 3 0 3 3	0 3 3 0 3 3 0	0 0 4 0 0	3 3 0 3 3	3 3 0 3 3	0 0 1 0	÷ 16
	1 -	_	2 1		2 1		-				3 0				0 1	

Note once again the multipliers 2 or 0 only in the interior in the first case.

9. Numerical Illustrations and Comments. We consider the application of the formulas to two examples: (i)  $f(x, y) = \cos x \cos y$ ; and (ii)  $f(x, y) = \sin x \sinh y$ , a harmonic function.

(i) 
$$I = \int_{-1}^{1} \int_{-1}^{1} \cos x \cos y \, dx \, dy = 4 \sin^2 1$$
  
hence  $\frac{1}{4}I = 0.708073.$ 

whence

The series (5.4) gives

fo	1	.000000
$\nabla^2 f_0/3!$	—	.3333333
$\nabla^4 f_0/5!$	+	33333
$4  \mathfrak{D}^4 f_0 / 3 \cdot 5!$	+	11111
$ abla^6 f_0/7!$	_	1587
$4 \mathfrak{D}^4 \nabla^2 f_0 / 7!$	_	1587
$\nabla^8 f_0/9!$	+	44
8 $\mathfrak{D}^{4} \nabla^{4} f_{0}/9!$	+	88
$16 \ \mathfrak{D}^{8} f_{0} / 5 \cdot 9!$	+	9
$\mathbf{Sum}$	0	.708078

This indicates the need for another term, and the alternation in sign, in this case, of terms with successive powers of  $h^2$ .

Table I shows the results of applying various formulas, with various values of h. Results are given to 5 decimals (based on calculations with 6-decimal function values). The column  $\epsilon$  gives the error (formula—true value) and column C gives the computed value of the leading correction term, as listed in earlier paragraphs;  $\epsilon$  and C are in units of the 5th decimal.

Formula		h = 1			h = 1/2	k = 1/3		
Tonnula	Result	e	C	Result	e	C C	Result	•
(A)	0.71701	+894	-1111	0.70858	+51	-53	0.70817	+10
(B) (C)	.72641 .62309	+1834 -8498	-2222 + 10000	.70909	$+102 \\ -462$	-107 + 481		
(D) (E)	.69353 .76398	-1454 + 5591	+1667 - 6667	.70730 .71114	-77	+80	0.70792	-15
(E) (G)	.72876	+3591 +2069	-2500	.70922	+307 +115	-320 - 120		
Formula		h = 2/3			h = 1/3			ý.
1 UIIIuia	Result	e	С	Result	e	с	-	
(A')	0.71199	+392	-494	0.70830	+23	-24	_	
(B') (C')	.71608	$+801 \\ -8819$	-988 +10617	.70852	+45 -488	-48 + 511		
(D') (E')	.70175 .74269	-632 + 3462	+741 -4198	.70773 .71000	-34 + 193	$+36 \\ -202$		
(Ĝ')	.71540	+733	-905	.70849	+42	-14		

TABLE I

	TABLE	Π
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Formula		h = 0.6		Formula	h = 0.4				
	Result	e	С	T OTHER	Result	¢	c		
(A) (B) (D) (E) (G)	$\begin{array}{c} 0.129414\\.129227\\.129879\\.128482\\.129181 \end{array}$	+187 0 +652 -745 -46	-186 -652 +745 +47	(A') (B') (D') (E') (G')	$\begin{array}{r} 0.129310\\.129227\\.129517\\.128689\\.129241 \end{array}$	$+83 \\ 0 \\ +290 \\ -538 \\ +14$	-83 -290 +538 -14		

We note that the correction estimate C is numerically larger than the actual error  $\epsilon$  in each case; this is due to the sign alternation mentioned earlier. We see also that, even with h = 1, C is quite a reasonable estimate of the size of  $\epsilon$ .

Formulas (C), (C'), as expected, are not very good. Formulas (E), (E'), are also poor, since  $\nabla^4 f_0$  and  $\mathfrak{D}^4 f_0$  have the same sign. The "product-Simpson" rule gives the best results—best of all with  $h = \frac{1}{3}$ . Formulas (D) and (D'), as exhibited in (F), (F') for a square of side 6h, suggest that (D) gives better results than (D') when the same points are used.

In practice, it is useful to use two formulas, and to compare results to give an estimate of the possible error. For this purpose (A) and (D) or (A') and (D') seem suitable pairs, unless it is known that f is harmonic or  $\nabla^4 f_0$  is expected to be small compared with  $\mathfrak{D}^4 f_0$ .

(ii)  $I = \int_0^{1,2} \int_0^{1,2} \sin x \sinh y \, dx \, dy = (1 - \cos 1.2)(\cosh 1.2 - 1) \approx 0.516908.$ 

Approximations to I/4 = 0.1292271 are listed; all 6 working decimals are shown in Table II. In this case, for a harmonic integrand, the superiority of (B) and (B') is evident; (G') is also good. In (B) and (B'), since  $\nabla^2 f_0 = 0$ , the error terms are of order  $h^8$  instead of  $h^4$ . The quadrature of a harmonic function will be considered further in a later note.

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1. W. G. BICKLEY, "Finite difference formulae for the square lattice," Quart. Jn. Mech. and Appl. Math., v. 1, 1948, p. 35-42.