**MLM-3787
UC-705**

Operational Equations for the Five-Point Rectangle

G. L. Silver

Issued: September 15, 1993

MOUND

operated by
EG&G MOUND APPLIED TECHNOLOGIES
P.O. Box 3000, Miamisburg, Ohio 45343-3000

for the
U. S. DEPARTMENT OF ENERGY
Contract No. DE-AC04-88DP43495

MASTER

ALL INFORMATION CONTAINED HEREIN IS UNCLASSIFIED

Contents

	Page
Abstract	3
Semiquadratic Interpolation on Five Points in Rectangular Array	4
First Exponential Method on Five Points in Rectangular Array	17
Application of Operational Formulas	22
References	34
Distribution	36

Abstract

Two operational polynomials are demonstrated for the four-point rectangle with center point. The equations are exact on the points and the surfaces they describe ordinarily fit known monotonic surfaces better than the standard five-point equation, as judged by the L_2 norm test. Equations for fitting the five-point rectangle by sines and cosines are presented.

Semiquadratic Interpolation on Five Points in Rectangular Array

The principles of the operational method for data interpolation were presented in 1985 [1]. The technique is an extension of Heavisidean operator methods. Although the calculus of operations was apparently known to Leibnitz, Heaviside's name has become associated with the subject because he used it in the study of electrical phenomena. An interesting book that describes some of the principles of the operational calculus, as well as Heaviside's unhappy life, was published a few years ago [2]. Chapter 10 focuses on operational methods, although references to the subject occur throughout the book.

Operational methods for the interpolation of experimental data treat a variety of subjects such as fixed-point derivative formulas, fixed-point integration formulas, formulas connecting points in various two-dimensional designs, and formulas for three-dimensional configurations. The most interesting application, however, is the development of three methods for the interpolation of four data in rectangular array.

The four-point rectangle is widely used in experimental design methodology. The standard four-point, bilinear equation commonly used to interpolate these rectangles tends to be a poor predictor. The three operational methods are usually better predictors than the bilinear equation, at least as judged by standards such as center point comparisons and the square of the L_2 norm test. This applies primarily to data that are monotonic increasing or monotonic decreasing in both the x and y directions, although operational equations are not restricted to such data. In other words, the operational equations apply principally to data that do not contain an interior extremum, a ridge, or a trough.

Interpolation of five-point rectangles, where the fifth point is the center point of the rectangle, is not a subject that is widely discussed. It was mentioned in Reference 3, in the section titled *Rectangles with More Than Four Points*. Reference 3 contains two equations for the five-point rectangle, but those are not the only equations that could have been suggested. The form of the polynomials that can be used for the five-point rectangle is given as Equation 1 below.

$$z = CN + (XC)x + (YC)y + (XYC)xy + (X2)x^2 + (Y2)y^2 \quad (1)$$

In Equation 1, the term CN is the constant term, XC is the coefficient of the linear term, x, and X2 is the coefficient of the quadratic term, x^2 . A similar convention applies to the other independent variable, y. XYC is the coefficient of the "interaction" term.

Equation 1 applies to the rectangle shown in Figure 1 below; measurements are taken at points A, C, E, G, and I. The following coefficients apply in the -1...1 coordinate system, so that the coordinates of center point E are (0,0). In the tests to be described, Figure 1 is filled with the nine successive integers 1 through 9 at the designated points A through I, respectively.

G	H	I
D	E	F
A	B	C

Figure 1 - Nine-Point Rectangle.

$$\begin{aligned}
\text{CN} &= \text{E} & (2) \\
\text{XC} &= (1/4)(\text{I} + \text{C} - \text{A} - \text{G}) & (3) \\
\text{YC} &= (1/4)(\text{I} + \text{G} - \text{A} - \text{C}) & (4) \\
\text{XYC} &= (1/4)(\text{I} + \text{A} - \text{C} - \text{G}) & (5) \\
\text{X2} &= (1/8)(\text{A} + \text{C} - 4\text{E} + \text{G} + \text{I}) \\
&\quad (-/+)(1/4)[\text{SQRT}(\text{C} - 2\text{E} + \text{G})][\text{SQRT}(\text{A} - 2\text{E} + \text{I})] & (6) \\
\text{Y2} &= (1/8)(\text{A} + \text{C} - 4\text{E} + \text{G} + \text{I}) \\
&\quad (+/-)(1/4)[\text{SQRT}(\text{C} - 2\text{E} + \text{G})][\text{SQRT}(\text{A} - 2\text{E} + \text{I})] & (7)
\end{aligned}$$

Or:

$$\begin{aligned}
\text{X2} &= (1/8)(\text{I} - \text{G} - \text{A} + \text{C})^2(\text{I} + \text{A} + \text{G} + \text{C} - 4\text{E}) \\
&\quad /[(\text{I} - \text{A})^2 + (\text{C} - \text{G})^2] & (8) \\
\text{Y2} &= (1/8)(\text{I} + \text{G} - \text{A} - \text{C})^2(\text{I} + \text{A} + \text{C} + \text{G} - 4\text{E}) \\
&\quad /[(\text{I} - \text{A})^2 + (\text{C} - \text{G})^2] & (9)
\end{aligned}$$

The coefficients XC, YC, and XYC are the same as similar coefficients for the standard bilinear equation on the four corner points A, C, G, and I. The two operational polynomials for the five-point rectangle have different coefficients for the squared terms, however [3].

Another set of coefficients for the X2 and Y2 terms in Equation 1 is given as Equations 10 and 11. The three six-term equations that can be derived from these coefficients illustrate that alternative methods for the five-point rectangle can be constructed. If the arguments of adjacent square root operators are negative, such as might occur in Equations 6 and 7, they combine to yield a negative number. This accords with the custom for the imaginary operator: $i^2 = -1$.

$$\begin{aligned}
X2 = & [A^3 - A^2(C + 4E - 3G + I) + A(C^2 + 2C(G - I) + 8EI - 3G^2 \\
& - I(2G + I)) - C^3 + C^2(4E + G - 3I) - C(8EG - G^2 - I(2G \\
& + 3I)) + (G - I)(4E(G + I) - G^2 - I^2)] / [8(A - C + G - I) \\
& (A + C - G - I)]
\end{aligned}
\tag{10}$$

$$\begin{aligned}
Y2 = & [A^3 + A^2(3C - 4E - G - I) - A(3C^2 + 2C(I - G) - 8EI - G^2 \\
& + I(2G + I)) - C^3 + C^2(4E + G + I) - C(8EG - G^2 + I(I - 2G)) \\
& + (G - I)(4E(G + I) - G^2 - I(4G + I))] / [8(A - C + G - I) \\
& (A + C - G - I)]
\end{aligned}
\tag{11}$$

The predictive powers of these three five-point polynomials tend to be better than the predictive powers of the standard bilinear equation that is used on four points in rectangular array. If care is exercised, the best of them seems to have the X2 and Y2 coefficients given as Equations 6 and 7, while the least desirable has X2 and Y2 coefficients given as Equations 10 and 11. This judgment is based on results of the L_2 norm test as well as the complicated forms of Equations 10 and 11.

For most purposes, the coefficients X2 and Y2 given as Equations 8 and 9 are the best selection. This judgment is based on the consequences of ambiguity and the results of applying the square of the L_2 norm test to tables of known functions. Where only qualitative comparisons are concerned, the square of the L_2 norm test is as indicative as the L_2 norm test itself. The square of this test is hereafter referred to simply as the L_2 norm test.

The polynomial that uses Equations 6 and 7 as the coefficients of its squared terms is not invariant under rotation unless allowance is made for the ambiguity of signs connecting the terms in each of these coefficients. The ambiguity arises because square roots can be either positive or negative. Stated otherwise, the coefficients of the squared terms in the numerical interpolating polynomial may require transposition.

One way to deal with the ambiguity is to use Equations 8 and 9 as a guide; these latter equations determine the correct order by analogy. That is, if X^2 is larger than Y^2 in Equations 8 and 9, the same order usually prevails in Equations 6 and 7. Another way is to examine the behavior of both polynomials that derive from Equations 6 and 7, and then discard the inappropriate one. The ambiguity of the signs in Equations 6 and 7 is troublesome and inconvenient. These coefficients can yield a more accurate interpolating polynomial, but they need special attention because they may require transposition to obtain that polynomial. Equations 8 and 9 do not present this difficulty, so they will probably be preferred in most applications.

Equations 6 and 7 were also presented in Reference 3 as Equations 26 and 27. The minus and plus signs in those equations, respectively, can be retained if the arguments of adjacent square root operators are multiplied together under one common square root operator. Although this change does not obviate the need for the comparison test, it will be found to be useful in many practical applications that involve programming languages like BASIC. Computer algebra programs may force the separation of arguments so that the forms of Equations 6 and 7 cannot be avoided.

Table 1 presents the results of the L_2 norm test using the standard bilinear equation on four points, as well as the similar results obtained using Equation 1 as substituted with the coefficients given as Equations 2 through 5 and 8 through 9, above. When the L_2 norm test, or its square, yields zero as its result, the true surface and the approximating surface coincide exactly. The closer the result of the L_2 norm test is to zero, the "closer" the approximating surface is to the true surface. Table 1 illustrates that the operational equation fits the sample of known surfaces as well as or better than the standard bilinear equation.

Table 1. RESULTS OF L_2 NORM TEST ON SOME SIMPLE FUNCTIONS

Test Function	Bilinear Equation	Five-Point Equation
$(5 + x + 3y)$	0.0	0.0
$(5 + x + 3y)^2$	206.9	0.0
$\text{SQRT}(5 + x + 3y)$	0.0487	0.00362
$1/(5 + x + 3y)$	0.140	0.0374
$1/(5 + x + 3y)^2$	0.283	0.106
$2^{(5 + x + 3y)}$	49654.0	8931.0
$(5 + x + 3y)^{(3/2)}$	6.48	0.0475
$(5 + x + 3y)^3$	47551.0	1010.0

The coordinate system used in this table is -1...1. The five-point equation is Equation 1 substituted with the coefficients given in Equations 2 through 5 and 8 through 9.

It is possible to view the matter of polynomials for five-point rectangles from another perspective. The general form of the polynomial is given by Equation 1 above, and the coefficients CN, XC, YC, and XYZ are given in Equations 2 through 5, respectively. However, the coefficients X2 and Y2 are changed. They become:

$$X2 = (1/4)(A + G + I + C - 4E) - V \quad (12)$$

$$Y2 = V \quad (13)$$

In Equations 12 and 13, V is an independent variable. As a practical matter, the value of V that minimizes the result of the L_2 norm test is sometimes close to that value predicted by Y2 in Equation 7. In other words, Equations 6 and 7 may present some advantage in accuracy, compared to Equations 8 and 9, if the ambiguity of signs in Equations 6 and 7 can be resolved.

Table 2 is an attempt to clarify these observations by citing illustrative data derived from three rapidly ascending surfaces that are monotonic increasing in both the x and y directions.

Table 2. THREE ILLUSTRATIONS OF THE V VALUE

Function	V from Equation 7	Optimum V
$2^{(5+x+3y)}$	110.3 (8798)	108.2 (8795)
$(5+x+3y)^3$	135.0 (990.5)	135.0 (990.5)
$(5+x+3y)^4$	1458 (400099)	1452.3 (400080)

The coordinate system in Table 2 is -1...1. The value of V in the middle column was calculated from Equation 7. Values in parentheses are the values of the square of the L_2 norm test at the designated value of V. The results in the right hand column are based on the true function in the left hand column and the five-point interpolating equation that uses V as an independent variable. (See Equations 12 and 13.) Near the optimum value of V, the result of the L_2 norm test passes through a minimum. The data are monotonic increasing in both the x and the y directions.

To illustrate how one of the operational, five-point equations approximates the results obtained by the popular least squares, nine-point equation, it is instructive to compare the numerical values of the coefficients obtained by them. The selected operational equation is Equation 1 substituted by Equations 2 through 5 and 8 through 9. The comparison is shown for some simple functions in Table 3.

Table 3. COEFFICIENTS OF THE SIX-TERM EQUATION OBTAINED BY ONE OF THE FIVE-POINT OPERATIONAL POLYNOMIALS AND THE NINE-POINT LEAST SQUARES POLYNOMIAL FOR SOME SIMPLE FUNCTIONS

Function	CN	XC	YC	X2	Y2
$5 + x + 3y$	5.0	1.0	3.0	0.0	0.0
	5.0	1.0	3.0	0.0	0.0
$(5 + x + 3y)^2$	25.0	10.0	30.0	1.0	9.0
	25.0	10.0	30.0	1.0	9.0
SQRT(5+x+3y)	2.236	0.272	0.728	-0.017	-0.124
	2.243	0.256	0.721	-0.022	-0.125
1/SQRT(5+x+3y)	0.447	-0.117	-0.217	0.028	0.097
	0.432	-0.093	-0.203	0.030	0.106
Ln(5+x+3y)	1.609	0.337	0.761	-0.049	-0.250
	1.634	0.293	0.738	-0.057	-0.260
$(5+x+3y)^{(3/2)}$	11.18	3.17	9.83	0.165	1.58
	11.17	3.23	9.85	0.190	1.57

In Table 3, the coordinate system is $-1 \dots 1$. The polynomial used for comparison is Equation 1 substituted with the coefficients given as Equations 2 through 5 and 8 through 9. The coefficients CN , XC , YC , $X2$, and $Y2$ for this polynomial are listed as the first series of entries for each function. The second series of entries is the similar coefficients for the nine-point least squares polynomial. The coefficient XYC has the same value in both the operational and least squares equations.

Table 4 compares the fidelities of the four-point and five-point operational polynomial equations on some simple functions. The five-point equation is Equation 1 substituted with the coefficients given in Equations 2 through 5 and 8 through 9.

Comparison of the numbers in Table 4 with the analogous numbers in Table 1 shows that the improvement offered by the operational formulas, as judged by the L_1 norm test, occurs primarily when the standard bilinear equation for the four-point rectangle is replaced by the four-point operational, algebraic equation. If a rectangular surface must be represented in the form of an algebraic polynomial, there is usually some improvement on replacing the four-point operational algebraic equation with a well-chosen, five-point, operational algebraic equation, but the improvement is modest.

**Table 4. COMPARISON OF OPERATIONAL POLYNOMIAL EQUATIONS
FOR THE FOUR-POINT AND THE FIVE-POINT RECTANGLES**

Function	Four-Point Equation	Five-Point Equation
$5 + x + 3y$	0.0	0.0
$(5 + x + 3y)^2$	0.0	0.0
$\text{SQRT}(5+x+3y)$	0.00356	0.00362
$1/(5+x+3y)$	0.0414	0.0374
$1/(5+x+3y)^2$	0.113	0.106
$2^{(5+x+3y)}$	11470.0	8931.0
$\ln(5+x+3y)$	0.0340	0.0323
$(5+x+3y)^3$	1739.0	1010.0
$(5+x+3y)^{(3/2)}$	0.0581	0.0475

In Table 4, the four-point operational equation is Equation 9 in Reference 4. The five-point operational equation is Equation 1 above substituted with the coefficients given as Equations 2 through 5 and 8 through 9. The coordinate system is -1...1. The numbers are the results of the square of the L_2 norm test using the functions and equations as indicated.

It was observed in Reference 3 that the five-point interpolating equation containing coefficients, given as Equations 22 through 27 therein, should be abandoned if the coefficients are complex numbers. If the imaginary parts of the coefficients are discarded, but the real parts are retained, an acceptable interpolating equation is obtained in many cases.

This equation is the standard equation on five points in rectangular array. It can be as good as an operational equation for many practical purposes. This bears out the observation that, the more points there are involved, the smaller the advantage of the operational methods over standard methods.

The standard equation for five points in rectangular array is encountered much less frequently than the standard equation for four points in rectangular array. The standard five-point equation takes the form of Equation 1 and has the coefficients CN, XC, YC, and XYZ as listed in Equations 2 through 5 respectively. The coefficients X2 and Y2 are identical, however. They are:

$$X2 = Y2 = (1/8)(A + C - 4E + G + I) \quad (14)$$

Table 5 compares the standard five-point equation to Equation 1 when that equation is substituted with the coefficients given as Equations 2 through 5 and 8 through 9. It can be surmised from this table that the operational equation is often a better predictor than the standard equation, but that the advantage need not be substantial.

Table 5. COMPARISON OF THE STANDARD FIVE-POINT EQUATION TO AN OPERATIONAL FIVE-POINT EQUATION

Function	Standard Equation	Operational Equation
$5 + x + 3y$	0.0	0.0
$(5 + x + 3y)^2$	11.38	0.0
$\text{SQRT}(5+x+3y)$	0.00545	0.00362
$1/(5+x+3y)$	0.0390	0.0374
$1/(5+x+3y)^2$	0.107	0.106
$2^{(5+x+3y)}$	10106.0	8931.0
$\ln(5+x+3y)$	0.0392	0.0323
$(5+x+3y)^3$	3550.0	1010.0
$(5+x+3y)^{(3/2)}$	0.383	0.0475

The coordinate system in Table 5 is -1...1. The numbers in the columns represent the square of the L_2 norm test using the indicated functions. The standard equation uses X2 and Y2 coefficients as indicated in Equation 14, and the operational equation uses these coefficients as indicated in Equations 8 and 9, respectively.

First Exponential Method on Five Points in Rectangular Array

The first exponential method of operational interpolation on four points in rectangular array can be applied as a computer program in BASIC language [5], or in an abbreviated form suitable for programmable calculators and symbolic mathematics packages [6]. The latter approach permits the substitution of expressions for side points B and D into the equation that is used for the interpolation. This convenience permits the expression to be based on five points in rectangular array, where the fifth point is the center point of the rectangle. Expressions for side points B and D are as follows:

$$B = (1/2)(C + A)[\text{SQRT}(A + I + 2E)\text{SQRT}(2E + C + G) (+/-) \\ \text{SQRT}(A + I - 2E)\text{SQRT}(C + G - 2E)]/(A + C + G + I) \quad (15)$$

$$D = (1/2)(A + G)[\text{SQRT}(A + I + 2E)\text{SQRT}(2E + C + G) (-/+) \\ \text{SQRT}(A + I - 2E)\text{SQRT}(C + G - 2E)]/(A + C + G + I) \quad (16)$$

If the arguments of two adjacent square root functions are negative, they combine to yield a negative number. This may not be possible to execute on a pocket calculator without rewriting the equations. For example, multiply the arguments of adjacent square root operators under one common square root operator as described for Equations 6 and 7 above. The sign of this operator can be positive or negative.

Alternative side point expressions for the first exponential, operational equation are:

$$\begin{aligned}
 B = & [\text{SQRT}(2)/2](C + A)\text{SQRT}[(G^2 - C^2)(I - A) + (I^2 - A^2)(G - C) \\
 & + \text{SQRT}[(2(C + I - G - A)(C - I - G + A)E)^2 \\
 & + ((A - I)(C - G)(A + C + I + G))^2]] \\
 & /[(G - C + I - A)\text{SQRT}(A + C + G + I)]
 \end{aligned} \tag{17}$$

$$\begin{aligned}
 D = & [\text{SQRT}(2)/2](A + G)\text{SQRT}[(C^2 - G^2)(I - A) + (A^2 - I^2)(G - C) \\
 & + \text{SQRT}[(2(C - I - G + A)(G + A - I - C)E)^2 \\
 & + ((G - C)(A - I)(A + C + I + G))^2]] \\
 & /[(C + I - G - A)\text{SQRT}(A + C + G + I)]
 \end{aligned} \tag{18}$$

As often happens with formulas derived by the first exponential, operational method, Equations 15 through 18 should be restricted to data of one sign: positive data, ordinarily. Because of the ambiguity of sign that arises with the SQRT function, it may be desirable to use the absolute values of B and D. Note that Equations 15 and 16 both have an interior ambiguity of signs that needs resolution, as described above for the operational, five-point, algebraic method.

No equation for the five-point rectangle that derives from the second exponential method seems to be readily apparent, but neither is it apparent that this is an inherent limitation on that method. Empirical possibilities, however, include Equation 19:

$$P = J^*K^*M^z(E + Q) - Q \tag{19}$$

where the exponent z on M is taken as

$$z = (x^2 - 1)(y^2 - 1) \tag{20}$$

Equation 19 is solved as an empirical interpolating equation using the information at the five rectangle points A, C, G, I, and E. For example, consider a table of the squares of the first nine integers. In the -1...1 coordinate system, Equation 19 becomes:

$$P = 39.1918(1.2247)^x(2)^y(1.0206)^z - 15 \quad (21)$$

The constants in Equation 21 have been rounded to four decimal places. The equation fits the center and corner points of the table, as depicted in the diagram in the first section. On a similar table of the cubed integers, the interpolating equation is:

$$P = (136.3513)(1.4327)^x(3.8531)^y(1.0906)^z - 23.7 \quad (22)$$

Interestingly, both Equations 21 and 22 fit the tables that generated them better than the four-point, second exponential equations on the same data, respectively. The judgment "better than" is based on results of the L_2 norm test. Ordinarily, empirical methods are not preferred and are not used except as a last resort.

No reason has been given why the exponent z cannot assume other forms. In the -1...1 coordinate system, for example:

$$z = 1 - x^2/2 - y^2/2 \quad (23)$$

or

$$z = \cos[(x/2)Pi]\cos[(y/2)Pi] \quad (24)$$

Interpolating formulas so derived should be checked to ascertain that they reproduce the original data and that other desirable properties, such as invariance under rotation and translation, are maintained.

The interpolating equation for the second exponential method on the four-point rectangle can also be developed empirically; this yields an independent check on the operational calculus originally used to obtain that equation. The operational method has the advantage that it yields the form of the interpolating equation directly, something that must be assumed in the empirical approach. If this form $[P = J^*K^*(E + T) - T]$ is assumed to apply to arbitrary arrangements of four coplanar points, an empirical equation for these points is obtained in many cases. Thus, the second exponential method appears to be a general method that had its foundation in operational calculus, but which can be used quite apart from that approach if the generating equations can be solved. These observations also apply to three-dimensional applications.

Equation 19 can be rewritten as:

$$P = R(J^*)(K^*)(M^*) + Q \quad (25)$$

in which

$$J = \text{SQRT}(C - I) / \text{SQRT}(A - G) \quad (26)$$

$$K = \frac{(C + G - A - I)\text{SQRT}(G - I)}{[\text{SQRT}(C - I) - \text{SQRT}(A - G)][\text{SQRT}(C - I) + \text{SQRT}(A - G)]\text{SQRT}(A - C)} \quad (27)$$

$$M = \frac{[IA - CG + E(G + C - A - I)][\text{SQRT}(C - I) + \text{SQRT}(A - G)]}{[\text{SQRT}(C - I) - \text{SQRT}(A - G)]} \\ \frac{1}{[(A - G - C + I)\text{SQRT}(G - I)\text{SQRT}(A - G)\text{SQRT}(C - I)\text{SQRT}(A - C)]} \quad (28)$$

$$Q = (AI - CG) / (A - C + I - G) \quad (29)$$

$$R = \frac{[\text{SQRT}(G - I)\text{SQRT}(C - I)\text{SQRT}(A - C)\text{SQRT}(A - G)]}{[\text{SQRT}(C - I) + \text{SQRT}(A - G)][\text{SQRT}(A - G) - \text{SQRT}(C - I)]} \quad (30)$$

These formulas are so complicated that it is probably a mistake to routinely evaluate them in BASIC language; a computer program that can handle the square roots of negative numbers seems more appropriate. Even then, difficulties can arise if the sign of the square root is improper, so it may be better to solve all such problems using numerically substituted Equation 25 with a program for computer algebra. If complex numbers are generated, use the real parts of them.

Application of Operational Formulas

Suppose three counts representing the growth of bacteria at three equally spaced intervals are obtained. The bacterial counts, in arbitrary units, are 1, 2, and 20. The least squares straight line ($y = 9.5x - 1.833$) represents the counts rather poorly; it intersects none of the points, and predicts a negative count at time zero, whereas the true count was 1 arbitrary unit at the start of the experiment. Bacterial counts less than zero are impossible, so the straight line is not acceptable as a model of the system. A parabola ($y = 1 - 7.5x + 8.5x^2$) also predicts a negative count for part of the experiment, so it, too, is judged to be unacceptable. An exponential curve ($y = 0.9412 + 0.0588[(18^x)]$) gives a more reasonable representation of how the bacterial colony might be growing. It intersects all of the points, and is never negative in their domain.

Just as straight lines can misrepresent three curvilinear data, so can the standard bilinear model misrepresent four rectangular data. The standard bilinear model also uses straight lines. The analogy can be carried one more step; just as a parabola can misrepresent three curvilinear data, so can the operational algebraic model misrepresent four data in rectangular array. The algebraic model also uses parabolas [4,7].

When the linear and parabolic models of the three curvilinear data failed to yield acceptable representations, the next step was to try an exponential model. This reasoning carries over into two dimensions; the operational method yields two exponential models of four data in rectangular array. Ordinarily, the second exponential model [7] should probably be tried first. It is much simpler than the first exponential model, and it offers an alternative representation in some cases [3].

The operational method has provided three new equations for interpolating four data in rectangular array. With the possible exception of the first exponential equation [6], the operational equations share the virtue of simplicity with the standard bilinear equation. Compared to the bilinear equation, the operational equations have the additional virtue of fidelity on simple functions that do not contain an extremum like a ridge or a trough. This is usually borne out if the L_2 norm test is the criterion of merit.

It was observed in Reference 8 that operational four-point methods apply primarily to functions F whose first partial derivatives do not pass through zero more than once. Thus, not more than one member of the set of partial derivatives $\{dF/dx, dF/dy\}$ can be zero in the region to be interpolated, and that member cannot be zero more than once. For most practical applications of the four-point operational equations, no derivative should pass through zero in the region of interest.

Reference 6 includes a suggestion for estimating the center point of five ordered measurements. Using that suggestion, a quadratic equation must be solved. For an odd number of data, N , it is much easier to evaluate the center point on $N-1$ of them, where the removed datum is the median of the set. The operational algebraic center point of the original set then becomes the arithmetic average of this median and the center point as estimated by the operational algebraic formula on the $N-1$ remaining data. This method has the advantages of simplicity and avoiding the ambiguity presented by a quadratic equation. It can also be generalized to any odd number of data.

Seven data can be contrived for which the quadratic equation method yields numbers that seem unreasonable as center point estimates. For example: 2, 4, 8, 16, 20, 24, and 28. Thus, whatever the merits of the quadratic equation method on five ordered data, it does not seem to permit

generalization to higher numbers of measurements. Intuition, historically an influence on the selection of center point estimators [9], is not abused if the quadratic equation method is avoided.

For an odd numbered set of ordered data of one sign, remove the median of the set. Multiply this median by the first exponential, center point estimate on the $N-1$ remaining data. The operational first exponential estimate of the center point of the original set is the square root of this product. The outlined procedure has the advantage that an estimate of the center point on a set of five ordered data can also be obtained by the second exponential method: treat the data as above for the first exponential method.

The method of estimating the center point (or the central tendency) of any ordered data by the use of formulas originally applicable to even numbers of data was first suggested in Reference 10. The technique has the advantage of robustness in the sense that it is not usually as sensitive to an "outlier" as the arithmetic average. In fact, the predicted value of the center point of ordered data often moves away from an outlier as the aberrancy of the outlier increases. On an even number of ordered data, the rationale for the procedure is the supposition of a relationship between a function and its increments [6]. For an odd number of data, the last step is a correction for the imperfect nature of the supposition. Although the method appears to be suitable for any number of ordered measurements, it becomes unwieldy for more than nine of them. In that case, a routine can be prepared that automatically generates the appropriate formulas from the number of input data. As is usual for first exponential formulas, they are not invariant under translation and apply only to data of one sign.

Applications of operational formulas include the solution of partial differential equations over specified regions. For example, Blakey and Hutton [11] have described the solution of the partial differential equation:

$$d^2f/dx^2 + d^2f/dy^2 + 4x^2y^2 = 0 \quad (31)$$

over the rectangular grid in the closed intervals 0...5 for x and 0...4 for y, the boundary conditions being zero. (The letter "d" stands for partial differentiation in Equation 31.) The solutions to Equation 31 in the rectangular region are given in the Table 6.

Table 6. SOLUTIONS OF EQUATION 31 USING EQUATION 32

59.95	142.39	230.14	251.62
61.41	135.47	202.56	200.34
34.23	71.50	100.31	91.16

The foregoing solutions depend upon the standard formula for the second derivative on three equidistant points B, C, and D:

$$C'' = (D - 2C + B)/(h^2) \quad (32)$$

Equation 32 is not the only formula for the second derivative at C that can be proposed. A host of operational second derivative formulas might have been selected instead. For example:

$$C'' = [(D + B)^4/16 - (D + B)^3C + (15/4)(C^2)(D + B)^2 + 4C^3(D+B) - 16C^4]/(9C^3h^2) \quad (33)$$

Equation 33 is obtained from Equation 14a in Reference 12. As can be discerned from that reference and other monographs on operational methods, Equation 33 is only one selection among many possibilities provided the operational method of data treatment.

The solution table provided by Equation 33 is given in Table 7.

Table 7. SOLUTIONS OF EQUATION 31 USING EQUATION 33.

58.36	139.73	226.49	248.17
59.90	132.78	198.79	196.72
33.47	70.10	98.30	89.16

The numbers in Tables 6 and 7 are presented with greater precision than is warranted by Equations 32 and 33, but the extra precision helps to contrast the tables. The solution tables show similar numbers, and numbers that change in about the same pattern. The question arises: should the standard formulas be used in the tabular solution of differential equations, or should operational formulas be used? If the latter, which operational formulas?

These questions are partly answered by examination of the differential equation. If it generates data of mixed signs, the standard derivative formulas should be used. If the differential equation generates data of one sign, and this data is generated by a linear or quadratic part, as in Equation 81, the standard derivative formulas also seem to be indicated. However, if the part that generates the numbers has a transcendental form, an operational formula might be desirable. The selection of operational derivative formulas must then be made.

Operational derivative formulas tend to be more complicated than the standard derivative formulas. Systems of simultaneous equations should be uncomplicated or they may not be solvable by commercial computer algebra programs. In other words, considerations of accuracy on known functions are subordinate to considerations of practicality. Additionally, it is an assumption that a system of equations based on operational derivative formulas has a solution. Whatever the selection of derivative formulas, however, the tabular solution of differential equations by large numbers of simultaneous equations is a tedious and error-prone procedure.

In Reference 3, the method of quadrants was described as substituting equations for points. The part of the equation containing the experimental data is substituted for a point, not the complete equation, including the sign of equality. In Reference 13, the observation about superposition of equations on page 22 refers to equations of different origins combined with the least squares technique.

An operational interpolating equation for the eight-point star design with an additional point at the center can be prepared. The eight peripheral points form an octagon, and the ninth point is at the center of the octagon. The octagon sits upon vertex B and has vertex H at its apex. It looks like a nine-point square with points B, F, H, and D pulled outward from lines AC, CI, IG, and GA, respectively. Take an operational equation for the five point rectangle. Choose the quadratic coefficients as Equations 8 and 9, for example. This is the first operational polynomial; it is expressed in terms of the square with corner values A, C, I, and G in a counterclockwise sense. Next, rotate the square so that it has corner values B, F, H, and D. The second operational polynomial is calculated to fit this square.

For purposes of tests, A, C, E, G, and I are functions of the integers 1, 3, 5, 7, and 9, respectively; whereas, B, D, F, and H are functions of $5-3[\text{SQRT}(2)]$, $5-[\text{SQRT}(2)]$, $5+[\text{SQRT}(2)]$, and $5+3[\text{SQRT}(2)]$, respectively. Test the first and second polynomials separately. Ascertain that they both operate properly on rectangular tables of bilinear numbers and the squares of bilinear numbers. Then take the arithmetic average of the two polynomials. This average is the desired equation for the star design; it is also exact on bilinear data and the squares of bilinear data in rectangular array.

The operational interpolating equation and the least squares equation for the same star design can be compared using the L_2 norm test within the limits -1...1 for both x and y. The operational equation often yields a slightly smaller number, indicating that the operational equation fits this section of the test surfaces slightly better than the least squares equation. However, the results are usually so close that the choice should be made on other grounds.

The least squares equation is closer to the corner points than the operational equation if the sum of the squares of the deviations is the criterion of merit, as is usually the case. This advantage, together with its long tradition, makes the least squares method a better selection than the cited operational equation for the star design. The operational equation for the star design also requires extrapolations for some of the points near the periphery of the star. Extrapolating is usually considered to be an undesirable procedure.

When the method of quadrants is applied to operational four-point interpolation formulas, new interpolation formulas for the nine-point rectangle are developed. It often happens that these operational nine-point formulas fit simple test surfaces better than the nine-point least squares formula. The judgment "better than" is based on the square of the L_2 norm test. But the L_2 norm test is not the only method for judging suitability or goodness of fit; another standard is the accuracy with which contour lines are forecast. By the latter criterion, the least squares equation is ordinarily superior to operational formulas. The least squares equation usually gives

reasonable estimates of contour lines if the data are not widely separated; additionally, its application for this purpose is traditional. Counterexamples are not hard to find, however.

In some branches of science, it is commonly supposed that effects diminish "as the inverse square of the distance." Let the test function, therefore, be $F(x,y) = 1/(1 + 2x + 6y)^2$ taken between the limits $x=0..1$ and $y=0..1$. Figure 2 plots the coordinates of the contour line corresponding to $F(x,y) - 0.02 = 0$. Near the top of the diagram are two closely spaced, almost parallel, downward sloping solid lines. The lower line of this pair represents the coordinates of the true contour line for $F(x,y) = 0.02$. The upper line of the pair represents the same line based on the second exponential, nine-point operational approximation to the surface $F(x,y)$. It can be seen from Figure 2 that the solid lines lie very close to one another. Figure 2 also contains two dashed lines: a short one above the aforementioned pair of solid lines, and a longer one lying substantially below the pair of solid lines. The dashed lines represent the least squares approximations to the coordinates of the contour line at the 0.02 level.

In this example, the least squares approximation to the level curve representing the response of 0.02 is inferior to the operational approximation. In the first place, the least squares method predicts two distinct lines when the function value is 0.02. This is misleading; the true function generates only one such line. Secondly, the least squares lines do not lie close to the true coordinates of the line representing the response 0.02. Thus, the second exponential, nine-point operational formula is superior to the least squares equation for two reasons. Although this example is illustrative, it does not address the problem of how to choose the best interpolation technique in laboratory situations.

Figure 2 - Coordinates of approximations to the contour line for the function $[1/(1 + 2x + 6y)^2 - 0.02 = 0]$.

Note: The coordinates of the true contour line and the contour line derived from the second exponential, operational nine-point approximation to the function are shown as the two closely spaced, nearly parallel solid lines. The two dashed lines are the least squares approximations to the coordinates of the true contour line.

The least squares method is so well established that hardly any other method is used for interpolating experimental data in two variables. Hunter uses the least squares method for studying carbon monoxide emissions [14]. Hunter's Figure 2 shows contour lines oriented along an axis about 135 degrees from the positive x_1 -axis. Does this mean that contour lines for CO emissions are really oriented along the 135 degree vector? No, it does not. Nature is not constrained by the method of least squares. The only way to be absolutely certain about the existence of contour lines, their shapes, and their orientations is to determine them experimentally.

The operational methods also indicate contour lines oriented along a vector approximately 135 degrees to the positive x_1 -axis. The operational response curves are not identical to the response curves obtained by the least squares method, but they are similar. Thus, all of the methods indicate comparable contour lines, more or less. The least squares method is advocated by tradition and especially by the popular dictum to believe in the simplicity of nature. This belief is contrary to human experience, however. Practically every phenomenon of nature has proven to be more complicated, upon closer examination, than was first suspected.

Draper and Lin [15] have presented criticisms of the algebraic operational equation for the four-point rectangle, Equation 2 in Reference 7. They state that the cited equation was derived by fitting a stationary ridge to the data as an assumption. The true origin of the cited equation is the center and side point formulas given in Reference 1. Those formulas were obtained by operational interpretation of trigonometric identities; geography had nothing to do with it.

Any equation that has the form of the cited operational equation presents an opportunity for a ridge or a trough. The presence of such a feature does not mean that it was the basis for developing the equation. Existence and causation are not synonymous. Contrary to Draper and Lin, ridges and eigenvalues played no assigned roles in deriving operational equations.

The bilinear equation uses a particular combination of four data. Each of the operational equations uses some other combination of the same data. The fundamental question is: What combination of the data is most advantageous for estimating values interior to the rectangle? Draper and Lin assume it is the combination found in the bilinear equation. They provide no reassurance by proof, by test, or by convincing argument. They do not suggest that context could influence the answer. They give no standard for superiority. The L_2 norm test is one criterion of merit, and by that criterion the operational equations are often superior to the bilinear equation [16].

REFERENCES

1. G. L. Silver, *Journal of Computational Chemistry*, 6:3 (1985), pp. 229-236.
2. P. J. Nahin, *Oliver Heaviside: Sage in Solitude*, The Institute of Electrical and Electronics Engineers, Inc., New York, 1987.
3. G. L. Silver, *Comparison of Operational and Standard Methods for Data in Rectangular Array*, MLM-3773, EG&G Mound Applied Technologies (February 1993), 28pp. (This reference gives some descriptive information about the L_2 norm test.)
4. G. L. Silver, *Operational Surfaces for the Rectangle and Triangle*, MLM-3748 (June 1992), 41 pp.
5. G. L. Silver, *Operational Interpolation of Data in Triangular Array*, MLM-3689 (May 1991), 35 pp.
6. G. L. Silver, *Three-Dimensional Operational Interpolation*, MLM-3722 (December 1991), 53 pp. (This report contains an application of MacLaurin's series. The essence of the subject can be found in a book published more than 150 years ago: *The Differential and Integral Calculus*, by A. DeMorgan, Baldwin and Craddock, London, 1842. See page 646. The application would have been of no interest were it not another connection between the first exponential and the algebraic operational methods. Its appearance in DeMorgan's book implies an earlier origin; this gives some idea of the state of development of operational calculus before the birth of Heaviside.)
7. G. L. Silver, *Quality Engineering*, 4 (1991-2), pp. 57-61.
8. G. L. Silver, *Mound Activities in Chemical and Physical Research: January-December 1991*, MLM-3768 (November 1992), see page 6.
9. W. C. Waterhouse, *Archive for History of the Exact Sciences*, 41:1 (1990), pp. 41-52.

10. G. L. Silver, *Operational Measures of Central Tendency*, MLM-3598 (August 1989), 28 pp.
11. J. Blakey and M. Hutton, *Engineering Mathematics*, Blackie and Son, Limited, London, 1960. (See section 8 in Chapter 18, p. 531.)
12. G. L. Silver, *Extensions of the Operational Method*, MLM-3382 (August 1986), 29 pp.
13. G. L. Silver, *Operational Methods for Data Interpolation*, MLM-3277 (August 1985), 37 pp.
14. J. S. Hunter, *Quality Engineering*, 1(4) (1989), pp. 453-465.
15. N. R. Draper and D. K. Lin, *Quality Engineering*, 5 (1993) pp. 369-373.
16. G. L. Silver, *Quality Engineering*, 6 (1993) 307-310. (In this manuscript, the "familiar nine-point method" is the least squares nine-point method.)

Distribution

External

OSTI, UC-705 (98)

S. N. Deming, Chemistry Department, University of Houston

W. Dyksen, Computer Science Department, Purdue University

E. Gartland, Department of Mathematical Sciences, Kent State University

J. S. Hunter, Princeton NJ

L. D. Kirkman, DAO/DOE

Internal

G. T. McConville

J. L. Clark

J. E. Riechers (2)

D. R. Rogers

G. L. Silver (4)

W. H. Smith

Document Control

Library (10)

Technical Publications

June E. Riechers, Editor
Technical Publications

END

**DATE
FILMED**

11 / 12 / 93