

NO FREE LUNCH: COMMENTS ON SILVER (1991-1992)

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Introduction

G. L. Silver recently sent us a copy of his 1991-1992 article in this journal and invited us to comment. His article appears at first sight to achieve the impossible, namely to estimate the six coefficients of a quadratic function in two predictors using just four data points. Silver does point out (p. 59) that "the coefficients must be related . . . and the relationship is not difficult to find," but then continues that this "has no immediate bearing on illustrating operational equations." It seems to us that it does have a bearing, in this sense: If we

understand the meaning of the relationships, we could then decide for ourselves whether using the method made any sense or not. We shall conclude below that it does not make sense, in general.

Connections Between the Operational Method of Silver and Standard Response Surface Methodology

Silver's (1991–1992) (1) article begins with a 2^2 grid of factorial response values:

$$\begin{array}{cc} G & I \\ A & C \end{array} \quad (1)$$

and suggests use of the quadratic equation

$$\hat{y} = A + (T2)x + (T4)y + (T1)x^2 + (T5)y^2 + (T3)xy \quad (2)$$

where

$$T1 = (A - C - G + I)(A - C + G - I)/[2(A + C - G - I)] \quad (3)$$

$$T2 = [2(A - C)(G + I) + (A + C)^2 + (G - I)^2 - 4A^2]/[2(A + C - G - I)] \quad (4)$$

$$T3 = (A - C - G + I) \quad (5)$$

$$T4 = [2(A - C)(G + I) + (A + C)^2 + (G - I)^2 - 4A^2]/[2(A - C + G - I)] \quad (6)$$

$$T5 = (A + C - G - I)(A - C - G + I)/[2(A - C + G - I)] \quad (7)$$

We see from Eq. (2) that when $x = y = 0$, $\hat{y} = A$. Thus the bottom corner is being used as an origin. Also if $x = 1$, $y = 0$, then

$$\hat{y} = A + T2 + T1 = C,$$

after much reduction. Similarly if $x = 0$, $y = 1$, $\hat{y} = G$ and finally, when $x = 1 = y$, $\hat{y} = I$. Thus Silver is working with a coding (0, 1) on each axis. We revert to the more usual coding (-1, 1), on each axis (see, e.g., Ref. 2, p. 308) via

$$x_1 = 2(x - 0.5) \quad x_2 = 2(y - 0.5) \quad (8)$$

or

$$x = (x_1 + 1)/2 \quad y = (x_2 + 1)/2 \quad (9)$$

and now substitute for Eqs. (3)–(9) into Eq. (2). A massive reduction, followed by identification of the usual regression coefficients

$$b_0 = (A + C + G + I)/4 \quad (10)$$

$$b_1 = (-A + C - G + I)/4$$

$$b_2 = (-A - C + G + I)/4$$

$$b_{12} = (A - C - G + I)/4$$

leads to the fitted model

$$\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + b_{12} x_1 x_2 + b_{11} (x_1^2 - 1) + b_{22} (x_2^2 - 1) \quad (11)$$

where

$$b_{11} = b_{12} b_1 / (2b_2) \quad b_{22} = b_{12} b_2 / (2b_1) \quad (12)$$

Note that, at the corners where $x_1 = \pm 1$, $x_2 = \pm 1$, the quadratic terms vanish, meaning that a model without pure quadratic terms is fitted to the actual data, while the quadratic coefficients b_{11} and b_{22} aid in providing interpolationary predictions at locations where there are no data. What kind of interpolations? If we were to determine the stationary point(s) of Eq. (11), subject to Eq. (12), we get two identical equations

$$X \equiv \frac{x_1}{b_2} + \frac{x_2}{b_1} + \frac{1}{b_{12}} = 0 \quad (13)$$

giving a line of stationary points. Defining

$$\underline{B} = \begin{pmatrix} b_{11} & \frac{1}{2}b_{12} \\ \frac{1}{2}b_{12} & b_{22} \end{pmatrix} \quad \underline{b} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \quad (14)$$

a common notation in this work (see, e.g., Ref. 3, p. 333) we find that the eigenvalues of \underline{B} are 0 and

$$\frac{1}{2}b_{12} \left[\frac{b_1^2 + b_2^2}{b_1 b_2} \right] \quad (15)$$

All this implies that a stationary ridge surface (see Figure 11.1(c), Ref. 3, p. 347) has been fitted to the data, a strong and usually unjustifiable assumption. Equation (11) can, in fact, be rewritten, with the help of Eqs. (12) and (13), as $X^2 = c$, where

$$c = \frac{2(\hat{y} - b_0)}{b_1 b_2 b_{12}} + \frac{1}{b_1^2} + \frac{1}{b_2^2} + \frac{1}{b_{12}^2} \quad (16)$$

For any given \hat{y} , c depends only on b_0 , b_1 , b_2 , and b_{12} which, in turn, depend only on the four observations through Eq. (10). Thus, for a given \hat{y} , the equation $X^2 = c$ defines the two lines $X = \pm\sqrt{c}$.

From all this, we see why there is no free lunch. In order to estimate the six coefficients of a quadratic model in (x_1, x_2) , Silver has used four pieces of information from the actual data (namely the A , C , G , and I values) and two

personally chosen extra conditions, which ensure that one eigenvalue of \tilde{B} is zero and that a line of centers is obtained, providing a stationary ridge type of fitted equation.

Any other assumptions can be investigated in a similar fashion. Suppose, for example, that b_1 and b_2 were interchanged in Eq. (12) so that we had chosen instead

$$b_{11} = b_{12} b_2 / (2b_1) \quad b_{22} = b_{12} b_1 / (2b_2) \quad (17)$$

This can, of course, also be described as an interchange of b_{11} and b_{22} . Then Eq. (11) can be rewritten as

$$\left[\frac{x_1}{b_1} + \frac{x_2}{b_2} + \frac{1}{b_{12}} \right]^2 = c \quad (18)$$

but the stationary point is at infinity. This gives us another limiting case, in which the response function consists of parallel straight lines with \hat{y} values increasing as we go towards the stationary point at infinity. Again, Eq. (18), like Eq. (16), is a special type of quadratic which arbitrarily adds two pieces of information to the four provided by the data.

One further point on Eq. (11). At $(x_1, x_2) = (0, 0)$, $\hat{y} = b_0 - b_{11} - b_{22}$. Thus under either set of assumptions, the prediction at the origin is "corrected" for the biases that would usually arise due to the fact that $E(b_0) = \beta_0 + \beta_{11} + \beta_{22}$, when the true model is quadratic. However, this correction is dependent on the specific assumptions.

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