

Response surface analysis incorporating neighbour effects from adjacent units

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ABSTRACT

The response surface analysis from a design with factorial treatment structure in which the experimental units exhibit the overlap effects from the neighbouring units has been dealt with. The analysis has been illustrated by fitting first order and second order response surfaces incorporating neighbour effects from adjacent units. The results show that if the neighbour effects are present and are included in the response model, there is a substantial reduction in residual sum of squares and the response is predicted more precisely. Besides, the parameters of the model are estimated with high precision.

Key words: Competition coefficient, Neighbour effects, Residual sum of squares, Response surface

Response surface methodology (RSM) consists of a set of techniques that includes setting up of an appropriately designed experiment, recording observations on the response of interest, estimating a model that best fits the collected data and determining the optimal settings of the experimental factors that produce the maximum (or minimum) value of the response. For example, RSM can be used to determine the optimum dose of nitrogen (N), phosphorous (P) and potash (K) for a crop to be recommended to farmers.

Let there be v input factors x_1, x_2, \dots, x_v and a response variable y . The response is a function of input factors, i.e.

$$y_u = f(x_{1u}, x_{2u}, x_{3u}, \dots, x_{vu}) + e_u \quad \dots(1)$$

where $u = 1, 2, \dots, n$ (n being the number of observations), x_{iu} is the level of the i^{th} factor, ($i = 1, 2, \dots, v$) in the u^{th} treatment combination, y_u denotes the response obtained from u^{th} treatment combination. The function f describes the form in which the response and the input variables are related and e_u is random error associated with the u^{th} observation which is assumed to be identically independently distributed normally with mean zero and common variance σ^2 . In practice, the form of f is not known and it is therefore approximated, within the experimental region by a polynomial of suitable degree in variables. Polynomials which adequately represent the true dose-response relationship are called response surface models and the designs that allow the fitting of response surfaces and provide a measure for testing their adequacy are called

response surface designs (Khuri and Cornell 1996).

In general, while carrying out response surface analysis, it is assumed that the observations are independent and there is no effect of neighbouring plots. But in many experiments this assumption seems to be unrealistic. In field experiments, the neighbour (interference or overlap or competition) effects from the treatments applied to the adjacent plots may arise. For example, if one plot receives a spray chemical treatment, wind drift may cause the effect of spray spill over to the adjacent plots. Therefore, it is more realistic to postulate that the response depend not only on the treatment combination applied to that particular plot but also depend on the treatments applied to the neighbouring plots. Hence, it is important to include the neighbour effects in the model to have the proper specification.

Draper and Guttman (1980) suggested a general linear model for response surface problems in which it is anticipated that the response on a particular unit will be affected by the treatments applied to the neighbouring units and the same has been illustrated. Sarika *et al.* (2009a) studied first order response surface model with neighbour effects from adjacent left and right neighbouring units and the conditions were derived for the orthogonal estimation of coefficients of this model and for constancy of the variances of the parameter estimates. Sarika *et al.* (2009b) studied second order response surface model with neighbour effects and the orthogonality conditions were derived. A method of obtaining designs satisfying the derived conditions was given.

In this paper, we have described the response surface analysis from a design with factorial treatment structure and in which the experimental units exhibit the overlap effects

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from the neighbouring units. The same has been illustrated through synthetic data sets. The competition coefficient, due to the neighbour effects, is estimated.

MATERIALS AND METHODS

Consider the model (1) where the response is a function of input factors, i e

$$y_u = f(x_u) + e_u, u=1, 2, \dots, n$$

where $x_u=(x_{1u}, x_{2u}, \dots, x_{vu})'$ defines the set of predictor values at which the response y_u is observed. If the function is a polynomial of degree one in predictor variable, it is called first order (linear) response surface, i e

$$f(x_u) = \beta_0 + \sum_{i=1}^v \beta_i x_{iu}$$

Following is a polynomial of degree two and is called second order (quadratic) response surface assuming the interaction to be absent:

$$f(x_u) = \beta_0 + \sum_{i=1}^v \beta_i x_i + \sum_{i=1}^v \beta_{ii} x_i^2$$

The model incorporating the neighbour effects from immediate neighbouring units can be written as:

$$y_u = \sum_{u'=1}^n g_{uu'} f(x_{u'}) + e_u \dots(2)$$

where,

$$\begin{aligned} g_{uu'} &= 1, \text{ if } u = u' \\ &= \alpha, \text{ if } |\alpha| < 1, \text{ if plots are physically adjacent} \\ &= 0, \text{ otherwise.} \end{aligned} \dots(3)$$

α is called the competition coefficient. It may be that all the neighbouring plots affect the response variable differently which results in increase in the number of parameters in the model and this in turn adversely affects the efficiency of estimation of the parameters. For all practical purposes, the present assumption of equal neighbour effects seems to be more appropriate.

When the response is a linear function of parameters, model (2) can be written as:

$$y = GX\beta + e \dots(4)$$

where y is a $n \times 1$ vector of observations on response variable, $G = (g_{uu'})$ is the $n \times n$ symmetric matrix of coefficient for neighbour effects, X is a $n \times p$ matrix of observations on predictor variables, β is a $p \times 1$ vector of parameters and e is a $n \times 1$ vector of uncorrelated errors that follows normal distribution with mean 0 and constant variance σ^2 .

If G is known, the least square estimate of β incorporating the neighbour effects is

$$\hat{\beta} = (X'G^2X)^{-1} X'Gy \dots(5)$$

with dispersion matrix,

$$D(\hat{\beta}) = \sigma^2 (X'G^2X)^{-1} \dots(6)$$

An unbiased estimate of error variance σ^2 is given by

$$\hat{\sigma}^2 = \frac{(y - GX\hat{\beta})'(y - GX\hat{\beta})}{n - p} \dots(7)$$

The first and second order response surface models have been fitted here as per specification (2) and the competition coefficient (α) in G is estimated such that the residual sum of squares (RSS) is minimum.

RESULTS AND DISCUSSION

Data set I: The data for a 2^3 factorial with 3 factors (say N, P and K) each at two levels (1, -1) along with layout is given in Table 1.

Table 1 Layout plan of 2^3 factorial with response, treatment combinations and plot numbers

26.57	56.14	61.03	53.79
(-1 -1 -1)	(-1 -1 1)	(-1 1 -1)	(-1 1 1)
Plot 1	Plot 2	Plot 3	Plot 4
30.51	56.26	67.02	56.58
(1 -1 -1)	(1 -1 1)	(1 1 -1)	(1 1 1)
Plot 5	Plot 6	Plot 7	Plot 8

Since there are eight observations, the 8×8 matrix of neighbour effects G as defined in (3) is obtained as:

$$G = \begin{bmatrix} 1 & \alpha & 0 & 0 & \alpha & \alpha & 0 & 0 \\ \alpha & 1 & \alpha & 0 & \alpha & \alpha & \alpha & 0 \\ 0 & \alpha & 1 & \alpha & 0 & \alpha & \alpha & \alpha \\ 0 & 0 & \alpha & 1 & 0 & 0 & \alpha & \alpha \\ \alpha & \alpha & 0 & 0 & 1 & \alpha & 0 & 0 \\ \alpha & \alpha & \alpha & 0 & \alpha & 1 & \alpha & 0 \\ 0 & \alpha & \alpha & \alpha & 0 & \alpha & 1 & \alpha \\ 0 & 0 & \alpha & \alpha & 0 & 0 & \alpha & 1 \end{bmatrix}$$

Plot 1 has plots 2, 5 and 6 as neighbouring plots, plot 2 has plots 1, 3, 5, 6 and 7 as neighbouring plots and so on. First order response surface model was fitted to these data with 3 factors. The RSS, coefficient of determination (R^2) and parameter estimates for different values of α were calculated. It is found that RSS is 675.091 at $\alpha = 0$ which decreases as α increases and is minimum (8.970) at $\alpha = 0.62$. Similar is the trend in case of R^2 values with minimum of 54.0% at $\alpha = 0$ and maximum of 99.4% at $\alpha = 0.62$. Thus, $\alpha = 0.62$. The fitted model with standard errors of estimates (in parenthesis) at $\alpha = 0$ is:

$$\hat{y} = 50.991^* + 1.604 N + 8.618 P - 4.705 K$$

(4.59) (4.59) (4.59) (4.59)

whereas at $\hat{\alpha} = 0.62$, it is:

$$\hat{y} = 14.654^* + 4.221^* N + 5.407^* P + 5.636^* K$$

(0.15) (1.39) (0.38) (1.33)

(* indicates statistical significance at $P = 0.01$).

Evidently, all the parameters except β_0 are not significant at $\alpha = 0$, whereas these parameters become significant at $\alpha = 0.62$, clearly indicating the impact of neighbouring units.

The variance of the estimated response at 2 sets of points in X is:

Table 3 Results of fitting second order model to data set II for different values of α

	α							
	0.0	0.4	0.6	0.8	0.83	0.84	0.85	0.9
RSS	982.046	342.704	214.711	71.050	67.244	66.893	66.961	72.715
R ²	0.8738	0.9560	0.9724	0.9909	0.9913	0.9914	0.9914	0.9907
$\hat{\beta}_0$	57.705 (3.568)	-9.083 (6.538)	38.706* (3.252)	28.990* (1.221)	27.848* (1.126)	27.472* (1.103)	27.099* (1.085)	25.291* (1.034)
$\hat{\beta}_1$	2.404 (1.652)	1.407* (0.568)	1.162* (0.371)	0.989* (0.182)	0.967* (0.173)	0.960* (0.171)	0.953 (0.170)	0.920 (0.171)
$\hat{\beta}_2$	8.470* (1.652)	2.441* (0.357)	1.704* (0.218)	1.309* (0.102)	1.267* (0.097)	1.253* (0.096)	1.240* (0.951)	1.180* (0.095)
$\hat{\beta}_3$	5.332* (1.652)	5.190* (1.016)	4.964* (0.767)	4.473* (0.406)	4.382* (0.390)	4.357* (0.387)	4.328* (0.385)	4.180* (0.391)
$\hat{\beta}_{11}$	-3.595 (2.861)	48.793* (10.703)	-31.900* (4.279)	-14.925* (1.034)	-13.853* (0.925)	-13.531* (0.894)	-13.225* (0.876)	-11.886* (0.809)
$\hat{\beta}_{22}$	-28.330* (2.861)	-10.838* (0.689)	-8.574* (0.439)	-7.199* (0.206)	-6.991* (0.194)	-6.923* (0.191)	-6.855* (0.189)	-6.525* (0.187)
$\hat{\beta}_{33}$	-0.440 (2.861)	-2.342 (3.112)	-9.866* (3.072)	-14.192* (1.541)	-13.902* (1.433)	-13.776* (1.408)	-13.635* (1.386)	-12.827* (1.332)

Figures within parentheses are the standard errors of the estimates
*P = 0.01

After estimating the parameters as per model (4), the least-squares residuals were subjected to run test in order to examine whether the errors were correlated. The test indicated that there was no evidence against the null hypothesis of observations being random (value of statistic, Z = 1.649, P = 0.099). This implied that inclusion of correlation among neighbouring units did not induce correlation among the observations. However, if the correlation is non-zero, then the generalized least-squares method may be adopted to estimate the parameters (for details see e.g, Johnston and Dinardo 2007).

Table 4 Layout plan of the experiment with treatment combinations and response

1	N ₁ S ₂ B ₂	18.51
2	N ₂ S ₀ B ₀	18.51
3	N ₁ S ₀ B ₀	18.64
4	N ₂ S ₁ B ₀	19.97
5	N ₁ S ₁ B ₀	20.14
6	N ₂ S ₂ B ₀	18.51
7	N ₁ S ₂ B ₀	21.42
8	N ₂ S ₀ B ₀	19.10
9	N ₁ S ₀ B ₁	18.95
10	N ₂ S ₁ B ₁	19.54
11	N ₁ S ₁ B ₁	26.82
12	N ₂ S ₂ B ₁	22.85
13	N ₁ S ₂ B ₁	26.82
14	N ₂ S ₀ B ₂	19.25
15	N ₁ S ₀ B ₂	19.68
16	N ₂ S ₁ B ₂	20.80
17	N ₁ S ₁ B ₂	18.65
18	N ₂ S ₂ B ₂	20.07

Data set III: The data were taken from the experiment conducted on sunflower in 2005 by Agronomy Division of Indian Agricultural Research Institute, New Delhi. Two levels of N (uncoated and coated coded as 1 and 2, respectively), 3 levels of Sulphur, S (0, 25 and 50 kg/ha coded as 0, 1 and 2, respectively) and 3 levels of boron, B (0, 0.75 and 1.5 kg/ha

$$G = \begin{bmatrix} 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & & & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & & & & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & & & & & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & & & & & & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & & & & & & & & 1 & \alpha & 0 & 0 & 0 & 0 & 0 \\ & & & & & & & & & & & & 1 & \alpha & 0 & 0 & 0 & 0 \\ & & & & & & & & & & & & & 1 & \alpha & 0 & 0 & 0 \\ & & & & & & & & & & & & & & 1 & \alpha & 0 & 0 \\ & & & & & & & & & & & & & & & 1 & \alpha & 0 \\ & & & & & & & & & & & & & & & & 1 & \alpha \\ & & & & & & & & & & & & & & & & & 1 \end{bmatrix}$$

coded as 0, 1 and 2, respectively) resulting into 18 combinations were tested. This experiment was conducted in randomized block design with 3 replications. Here, we have considered replication 2 for illustration. The layout of this replication is given in Table 4.

The G matrix for this arrangement as defined in (3) is:

The quadratic model with interactions was fitted to the above data for different values of α . The fitted model with least value of RSS (43.011) and maximum value of R^2 (0.620) is seen to be:

$$\hat{y} = 16.204^* - 0.947N + 1.572^*S + 0.474B - 0.433NS + 0.875NB + 0.503SB - 0.320S^2 - 1.666^*B^2$$

(0.970) (0.830) (0.586) (0.494) (0.708) (0.869) (0.663) (1.054) (0.848)

at $\alpha = 0.2$, where figures in parentheses indicate the standard errors of the estimates. However, the fitted model at $\alpha = 0$ is

$$\hat{y} = 22.876^* - 0.613N + 1.171S - 0.019B - 0.409NS + 0.541NB - 0.391SB - 0.794S^2 - 2.834^*B^2$$

(1.224) (1.224) (0.671) (0.671) (0.671) (0.671) (0.821) (1.162) (1.162)

(* indicates statistical significance at $P = 0.05$).

with RSS = 48.578 and $R^2 = 0.571$. Thus $\hat{\alpha} = 0.2$. The coefficient of error variance in the variance of estimated response at the point, say (1 1 -1 -1 -1 -1 1 1 1) in X is 0.589 at $\hat{\alpha} = 0.2$ while it is 0.625 for the same point at $\alpha = 0$. Here, again the influence of neighbour plots are marked and

thus should not be ignored. The optimum value of the input factors can similarly be obtained as in the case of data set II.

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