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Second-Order Response Surface Model with Neighbor Effects

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This article considers the second-order response surface model in which the experimental units, i.e., plots experience the neighbor effects from immediate left and right neighboring plots assuming the plots to be placed adjacent linearly with no gaps. Conditions have been derived for the estimation of coefficients of second-order response surface model. A method of constructing designs for fitting second-order response surface in the presence of neighbor effects has been developed. The designs so obtained are found to be rotatable.

Keywords Border plots; Neighbor effects; Response surface; Rotatable design; Second-order model.

Mathematics Subject Classification Primary 62K20; Secondary 62K15.

1. Introduction

Response surface methodology explores the relationship between response variable and several explanatory variables and the main idea is to obtain an optimal response using a set of designed points. A second-degree response surface in general is written as follows:

$$y_u = \beta_0 + \sum_{i=1}^v \beta_i x_{iu} + \sum_{i=1}^v \beta_{ii} x_{iu}^2 + \sum_{i=1}^{v-1} \sum_{i'=i+1}^v \beta_{i'i'} x_{iu} x_{i'u} + e_u,$$

where $u = 1, 2, \dots, N$ (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. β_0 is a constant, β_i is the i th linear regression coefficient, β_{ii} is the i th quadratic regression coefficient, and $\beta_{i'i'}$ is the (i, i') th interaction coefficient. e_u is the 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 . Details of response surface methodology can be seen in Box and Draper (1987), Myers and Montgomery (1995), and Khuri and Cornell (1996).

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In response surface methodology, it is assumed that the observations are independent and there is no effect of neighboring units. But in certain situations, this assumption seems to be unrealistic. For example, in field experiments, the neighbor effects from the treatments applied to the adjacent neighboring plots may arise. If one plot receives a spray chemical treatment, wind drift may cause the effect of spray spill over adjacent plots. Therefore, it is more realistic to postulate that the response depends not only on the treatment combination applied to that particular plot but also depends on the treatment combination applied to the neighboring 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 plot will be affected by overlap effects from neighboring plots and the same have been illustrated. Designs with neighbor effects for single factor in block design setup have been extensively studied in the literature (see, e.g., Azais et al., 1993; Jaggi et al., 2006; Tomar et al., 2005).

Here, we have studied the second order response surface model with no interaction terms in which the experimental plots exhibit the neighbor effects from immediate left and right neighboring plots assuming the plots to be adjacent linearly with no gaps. Interaction terms have not been considered because of complexity and analytical difficulties. Inclusion of interaction terms in the presence of immediate left and right neighbor effects does not permit to have neat expression for the estimates of parameters included in the model with their variance-covariance matrix. Conditions have been derived for the estimation of coefficients of second-order response surface model. A method of constructing designs for fitting second-order response surfaces in the presence of neighbor effects has also been developed and has been illustrated. The rotatable property of these designs has also been studied.

2. Second-Order Response Surface Model with Neighbor Effects

We consider here the following model (Draper and Guttman, 1980) with no interaction terms where the response is a function of input factors and incorporating the neighbor effects from immediate left and right neighboring plots:

$$y_u = \sum_{u'=1}^N g_{uu'} f(x_{u'}) + e_u, \quad (2.1)$$

where

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

and

$$\begin{aligned} g_{uu'} &= 1, & \text{if } u &= u' \\ &= \alpha, |\alpha| < 1, & \text{if } |u - u'| = 1, & \text{i.e., plots that are physically adjacent} \\ &= 0, & \text{otherwise.} \end{aligned} \quad (2.2)$$

It may be mentioned here that the layout of the experiment for estimating this model includes border plots for the end plots. The treatment combinations applied on them are the treatment combinations from the experiment. Observations for border plots are not modelled. Thus, Model (2.1) can be written as

$$Y = GX\beta + e, \tag{2.3}$$

where $G = ((g_{uu'}))$ is the $N \times (N + 2)$ neighbor matrix, X is a $(N + 2) \times (2v + 1)$ matrix of predictor variables and mean, β is a $(2v + 1) \times 1$ vector of parameters, and e is $N \times 1$ vector of errors which is $N(0, \sigma^2 I_N)$. If G is known, using Ordinary Least Squares (OLS) procedure, estimates of β 's are obtained as follows in the presence of neighbor effects:

$$\hat{\beta} = (Z'Z)^{-1}Z'Y, \tag{2.4}$$

where $Z = GX$ and $D(\hat{\beta}) = \sigma^2(Z'Z)^{-1}$

The $(N + 2) \times (2v + 1)$ matrix X of predictor variables and mean is written as:

$$X = \begin{bmatrix} 1 & x_{1N} & x_{2N} & \cdots & x_{vN} & x_{1N}^2 & x_{2N}^2 & \cdots & x_{vN}^2 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 1 & x_{11} & x_{21} & \cdots & x_{v1} & x_{11}^2 & x_{21}^2 & \cdots & x_{v1}^2 \\ 1 & x_{12} & x_{22} & \cdots & x_{v2} & x_{12}^2 & x_{22}^2 & \cdots & x_{v2}^2 \\ 1 & x_{13} & x_{23} & \cdots & x_{v3} & x_{13}^2 & x_{23}^2 & \cdots & x_{v3}^2 \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot \\ 1 & x_{1u} & x_{2u} & \cdots & x_{vu} & x_{1u}^2 & x_{2u}^2 & \cdots & x_{vu}^2 \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot \\ 1 & x_{1N} & x_{2N} & \cdots & x_{vN} & x_{1N}^2 & x_{2N}^2 & \cdots & x_{vN}^2 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 1 & x_{11} & x_{21} & \cdots & x_{v1} & x_{11}^2 & x_{21}^2 & \cdots & x_{v1}^2 \end{bmatrix}$$

The $N \times (N + 2)$ neighbor matrix G as defined in (2.2) is

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

Thus, $Z'Z$ is

$$\begin{bmatrix}
 N(1+2\alpha)^2 & (1+2\alpha)^2 \sum_{u=1}^N x_{1u} & (1+2\alpha)^2 \sum_{u=1}^N x_{2u} & \dots & (1+2\alpha)^2 \sum_{u=1}^N x_{vu} & \dots & (1+2\alpha)^2 \sum_{u=1}^N x_{2vu}^2 & \dots & (1+2\alpha)^2 \sum_{u=1}^N x_{vu}^2 \\
 (1+2\alpha^2) \sum_{u=1}^N x_{1u}^2 + A_1 & (1+2\alpha^2) \sum_{u=1}^N x_{1u} x_{2u} + C_{12} & (1+2\alpha^2) \sum_{u=1}^N x_{1u} x_{vu} + C_{1v} & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{1u}^3 + D_1 & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{1u} x_{2u}^2 + E_{12} & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{1u} x_{vu}^2 + E_{1v} \\
 (1+2\alpha)^2 \sum_{u=1}^N x_{2u}^2 + A_2 & (1+2\alpha)^2 \sum_{u=1}^N x_{2u} x_{vu} + C_{2v} & (1+2\alpha^2) \sum_{u=1}^N x_{2u} x_{vu}^2 + E_{2v} & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{2u}^3 + D_2 & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{2u} x_{vu}^2 + E_{2v} & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{2u} x_{vu}^2 + E_{2v} \\
 \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\
 (1+2\alpha)^2 \sum_{u=1}^N x_{vu}^2 + A_v & (1+2\alpha^2) \sum_{u=1}^N x_{vu} x_{2u}^2 + E_{v1} & (1+2\alpha^2) \sum_{u=1}^N x_{vu} x_{vu}^2 + E_{v1} & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{vu} x_{2u}^2 + E_{v2} & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^3 + D_v & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^3 + D_v \\
 (1+2\alpha^2) \sum_{u=1}^N x_{vu}^4 + B_1 & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^2 + B_1 & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^2 + B_1 & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^2 + B_1 & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^2 + F_{12} & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^2 + F_{1v} \\
 (1+2\alpha^2) \sum_{u=1}^N x_{2u}^4 + B_2 & (1+2\alpha^2) \sum_{u=1}^N x_{2u}^4 + B_2 & (1+2\alpha^2) \sum_{u=1}^N x_{2u}^4 + B_2 & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{2u}^4 + B_2 & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{2u}^4 + B_2 & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{2u}^4 + B_2 \\
 \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\
 (1+2\alpha^2) \sum_{u=1}^N x_{vu}^4 + B_v & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^4 + B_v & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^4 + B_v & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^4 + B_v & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^4 + B_v & \dots & (1+2\alpha^2) \sum_{u=1}^N x_{vu}^4 + B_v
 \end{bmatrix}$$

where

$$\begin{aligned}
 A_i &= 2\alpha^2 \left[\sum_{u=1}^N x_{iu} x_{i[(u+2) \bmod N]} \right] + 4\alpha \left[\sum_{u=1}^N x_{iu} x_{i[(u+1) \bmod N]} \right] \quad i = 1, 2, \dots, v \\
 B_i &= 2\alpha^2 \left[\sum_{u=1}^N x_{iu}^2 x_{i[(u+2) \bmod N]}^2 \right] + 4\alpha \left[\sum_{u=1}^N x_{iu}^2 x_{i[(u+1) \bmod N]}^2 \right] \quad i = 1, 2, \dots, v \\
 C_{ii'} &= \alpha^2 \left[\sum_{u=1}^N x_{iu} x_{i'[(u+2) \bmod N]} + \sum_{u=1}^N x_{i[(u+2) \bmod N]} x_{i'u} \right] \\
 &\quad + 2\alpha \left[\sum_{u=1}^N x_{iu} x_{i'[(u+1) \bmod N]} + \sum_{u=1}^N x_{iu} x_{i'[(u-1) \bmod N]} \right] \quad i \neq i' = 1, 2, \dots, v \\
 D_i &= \alpha^2 \left[\sum_{u=1}^N x_{iu} x_{i[(u+2) \bmod N]}^2 + \sum_{u=1}^N x_{iu}^2 x_{i[(u+2) \bmod N]} \right] \\
 &\quad + 2\alpha \left[\sum_{u=1}^N x_{iu} x_{i[(u+1) \bmod N]}^2 + \sum_{u=1}^N x_{iu}^2 x_{i[(u+1) \bmod N]} \right] \quad i = 1, 2, \dots, v \\
 E_{ii'} &= \alpha^2 \left[\sum_{u=1}^N x_{iu} x_{i'[(u+2) \bmod N]}^2 + \sum_{u=1}^N x_{i[(u+2) \bmod N]} x_{i'u}^2 \right] \\
 &\quad + 2\alpha \left[\sum_{u=1}^N x_{iu} x_{i'[(u+1) \bmod N]}^2 + \sum_{u=1}^N x_{i[(u+1) \bmod N]} x_{i'u}^2 \right] \quad i \neq i' = 1, 2, \dots, v \\
 F_{ii'} &= \alpha^2 \left[\sum_{u=1}^N x_{iu}^2 x_{i'[(u+2) \bmod N]}^2 + \sum_{u=1}^N x_{i[(u+2) \bmod N]}^2 x_{i'u}^2 \right] \\
 &\quad + 2\alpha \left[\sum_{u=1}^N x_{iu}^2 x_{i'[(u+1) \bmod N]}^2 + \sum_{u=1}^N x_{i[(u+1) \bmod N]}^2 x_{i'u}^2 \right] \quad i \neq i' = 1, 2, \dots, v.
 \end{aligned}$$

For the orthogonal estimation of parameters, $Z'Z$ has to be diagonal which is not feasible here for a second-order response surface model with neighbor effects because of some cross product terms. Hence, we try to obtain the diagonal matrix to the maximum extent possible, i.e., we try to make it nearly orthogonal so that some of the covariances are zero and others are constant. For obtaining this and for constancy of variances of linear parameters and quadratic parameters, the following conditions are required:

- i) $\sum_{u=1}^N \prod_{i=1}^v x_{iu}^{\omega_i} = 0$ for $\omega_i = 0, 1,$ or 3 and $\sum \omega_i \leq 3$
- ii) $\sum_{u=1}^N x_{iu}^2 = \text{constant} = N\eta = \delta \forall i = 1, 2, \dots, v$
- iii) $\sum_{u=1}^N x_{iu}^2 x_{i'u}^2 = \text{constant} = N\gamma = L$
- iv) $\sum_{u=1}^N x_{iu}^4 = \text{constant} = CL$
- v) $A_i = A, B_i = B$ and $F_{ii'} = F \forall i \neq i' = 1, 2, \dots, v.$ (2.5)

Therefore,

$$Z'Z = \left[\begin{array}{cc|c}
 N(1 + 2\alpha)^2 & \mathbf{0}'_{1 \times v} & (1 + 2\alpha)^2 \delta \mathbf{1}'_{1 \times v} \\
 \mathbf{0}_{v \times 1} & [(1 + 2\alpha^2)\delta + A] \mathbf{I}_v & \mathbf{0}_{v \times v} \\
 \hline
 (1 + 2\alpha)^2 \delta \mathbf{1}_{v \times 1} & \mathbf{0}_{v \times v} & \mathbf{H}_{v \times v}
 \end{array} \right]$$

with $\alpha \neq -0.5$ and

$$(\mathbf{Z}'\mathbf{Z})^{-1} = \begin{bmatrix} \frac{1}{N(1+2\alpha)^2} + v\frac{\delta}{N}\xi & \mathbf{0}'_{1 \times v} & -\xi\mathbf{1}'_{1 \times v} \\ \mathbf{0}_{v \times 1} & \frac{1}{[(1+2\alpha^2)\delta + A]}\mathbf{I}_v & \mathbf{0}_{v \times v} \\ -\xi\mathbf{1}_{v \times 1} & \mathbf{0}_{v \times v} & \Psi \end{bmatrix},$$

where,

$$\xi = \frac{\delta}{N} \left[\frac{[(1+2\alpha^2)L(C-1) + B - F] + (v-1)[(1+2\alpha^2)L + F - \frac{\delta^2}{N}(1+2\alpha)^2]}{\Delta} \right]$$

$$\Psi = \left[\frac{(1+2\alpha^2)L(C+v-1) + B + (v-1)F - v\frac{\delta^2}{N}(1+2\alpha)^2}{\Delta} \right] \mathbf{I}_v$$

$$- \left[\frac{(1+2\alpha^2)L + F - \frac{\delta^2}{N}(1+2\alpha)^2}{\Delta} \right] \mathbf{1}\mathbf{1}'$$

and

$$\Delta = [(1+2\alpha^2)L(C-1) + B - F] \times \left\{ [(1+2\alpha^2)L(C-1) + B - F] + v[(1+2\alpha^2)L + F - \frac{\delta^2}{N}(1+2\alpha)^2] \right\}.$$

Thus, variances of the estimates are

$$\left. \begin{aligned} V(\hat{\beta}_0) &= \frac{\sigma^2}{N(1+2\alpha)^2} [1 + v\delta(1+2\alpha)^2\xi] \\ V(\hat{\beta}_i) &= \frac{\sigma^2}{[(1+2\alpha^2)\delta + A]} \quad \text{for } i = 1, 2, \dots, v \\ V(\hat{\beta}_{ii}) &= \sigma^2 \left[\frac{(1+2\alpha^2)L(C+v-1) + B + (v-1)F - v\frac{\delta^2}{N}(1+2\alpha)^2}{\Delta} \right] \end{aligned} \right\}$$

with

$$\left. \begin{aligned} \text{Cov}(\hat{\beta}_0, \hat{\beta}_{ii}) &= -\sigma^2\xi \\ \text{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{i'i'}) &= -\sigma^2 \left[\frac{(1+2\alpha^2)L + F - \frac{\delta^2}{N}(1+2\alpha)^2}{\Delta} \right] \\ \text{Cov}(\hat{\beta}_0, \hat{\beta}_i) &= 0, \quad \text{Cov}(\hat{\beta}_i, \hat{\beta}_{i'}) = 0, \quad \text{Cov}(\hat{\beta}_i, \hat{\beta}_{ii}) = 0, \quad i \neq i' = 1, 2, \dots, v \end{aligned} \right\} \tag{2.6}$$

Here, the linear effects of all the factors are estimated orthogonal to all other effects. However, the quadratic effects are non orthogonal to mean effect and among themselves.

The estimated response at the point \mathbf{x}_0 is $\hat{y}_0 = \mathbf{x}'_0\boldsymbol{\beta} = \hat{\beta}_0 + \sum_{i=1}^v \hat{\beta}_i x_{i0} + \sum_{i=1}^v \hat{\beta}_{ii} x_{i0}^2$ with its variance

$$V(\hat{y}_0) = \mathbf{x}'_0 V(\hat{\boldsymbol{\beta}}) \mathbf{x}_0 = \sigma^2 \mathbf{x}'_0 (\mathbf{Z}'\mathbf{Z})^{-1} \mathbf{x}_0.$$

Thus,

$$\begin{aligned} V(\hat{y}_0) &= V(\hat{\beta}_0) + V(\hat{\beta}_i) \sum_{i=1}^v x_{i0}^2 + V(\hat{\beta}_{ii}) \sum_{i=1}^v x_{i0}^4 \\ &\quad + 2\text{Cov}(\hat{\beta}_0, \hat{\beta}_{ii}) \sum_{i=1}^v x_{i0}^2 + 2\text{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{i'i'}) \sum_{i=1}^{v-1} \sum_{i'=i+1}^v x_{i0}^2 x_{i'0}^2. \end{aligned}$$

Using (2.6) we get:

$$\begin{aligned} V(\hat{y}_0)\sigma^{-2} &= \frac{1}{N(1+2\alpha)^2} [1 + v\delta(1+2\alpha)^2\xi] \\ &\quad + \left\{ \frac{1}{[(1+2\alpha^2)\delta + A]} - 2\xi \right\} \sum_{i=1}^v x_{i0}^2 \\ &\quad + \frac{(1+2\alpha^2)L(C+v-1) + B + (v-1)F - v\frac{\delta^2}{N}(1+2\alpha)^2}{\Delta} \sum_{i=1}^v x_{i0}^4 \\ &\quad - 2\frac{[(1+2\alpha^2)L + F - \frac{\delta^2}{N}(1+2\alpha)^2]}{\Delta} \sum_{i=1}^{v-1} \sum_{i'=i+1}^v x_{i0}^2 x_{i'0}^2. \end{aligned}$$

If this variance is same for all points \mathbf{x} , then the design is said to be rotatable. The designs satisfying this property are called as Second Order Rotatable Designs with Neighbor Effects (SORDNE). We now present a method of constructing SORDNE.

3. Designs for Fitting Second-Order Response Model with Neighbor Effects

Construct a s^v ($s > 2$) full factorial for v factors each at s levels and arrange the combinations in lexicographic order starting from the highest order interaction and reaching to lowest one. Obtain $(v-1)s^v$ more combinations by circularly rotating the columns of s^v factorial such that each column occupies all the positions of the v columns. Two extra points are added as border plots for neighbor effects. The resulting design in vs^v points is a rotatable design for fitting second-order response model with neighbor effects. The design obtained here are found to be rotatable.

Example 3.1. Let $v = 2$ with each factor at three levels, then we get nine runs in full factorial. There are two columns for two factors, x_1 and x_2 . Next, we write the

contents of second column below first column and that of first column below second column. Finally, we add the first run at the bottom and last run at the top. The design matrix, X with 5 columns ($1 \ x_1 \ x_2 \ x_1^2 \ x_2^2$) and 18 points with two border points is as follows:

$$\mathbf{X} = \begin{bmatrix}
 1 & -1 & -1 & 1 & 1 \\
 1 & 1 & 1 & 1 & 1 \\
 1 & 0 & 1 & 0 & 1 \\
 1 & -1 & 1 & 1 & 1 \\
 1 & 1 & 0 & 1 & 0 \\
 1 & 0 & 0 & 0 & 0 \\
 1 & -1 & 0 & 1 & 0 \\
 1 & 1 & -1 & 1 & 1 \\
 1 & 0 & -1 & 0 & 1 \\
 1 & -1 & -1 & 1 & 1 \\
 1 & 1 & 1 & 1 & 1 \\
 1 & 1 & 0 & 1 & 0 \\
 1 & 1 & -1 & 1 & 1 \\
 1 & 0 & 1 & 0 & 1 \\
 1 & 0 & 0 & 0 & 0 \\
 1 & 0 & -1 & 0 & 1 \\
 1 & -1 & 1 & 1 & 1 \\
 1 & -1 & 0 & 1 & 0 \\
 1 & -1 & -1 & 1 & 1 \\
 1 & 1 & 1 & 1 & 1
 \end{bmatrix}$$

The 18×20 neighbor matrix G is defined as:

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

and

$$\mathbf{Z} = \mathbf{GX} = \begin{bmatrix} (1+2\alpha) & (1-\alpha) & 1 & (1+\alpha) & (1+2\alpha) \\ (1+2\alpha) & 0 & (1+2\alpha) & 2\alpha & (1+2\alpha) \\ (1+2\alpha) & (\alpha-1) & (1+\alpha) & (1+\alpha) & (1+\alpha) \\ (1+2\alpha) & (1-\alpha) & \alpha & (1+\alpha) & \alpha \\ (1+2\alpha) & 0 & 0 & 2\alpha & 0 \\ (1+2\alpha) & (\alpha-1) & -\alpha & (1+\alpha) & \alpha \\ (1+2\alpha) & (1-\alpha) & (-\alpha-1) & (1+\alpha) & (1+\alpha) \\ (1+2\alpha) & 0 & (-1-2\alpha) & 2\alpha & (1+2\alpha) \\ (1+2\alpha) & (\alpha-1) & -1 & (1+\alpha) & (1+2\alpha) \\ (1+2\alpha) & 1 & (1-\alpha) & (1+2\alpha) & (1+\alpha) \\ (1+2\alpha) & (1+2\alpha) & 0 & (1+2\alpha) & 2\alpha \\ (1+2\alpha) & (1+\alpha) & (\alpha-1) & (1+\alpha) & (1+\alpha) \\ (1+2\alpha) & \alpha & (1-\alpha) & \alpha & (1+\alpha) \\ (1+2\alpha) & 0 & 0 & 0 & 2\alpha \\ (1+2\alpha) & -\alpha & (\alpha-1) & \alpha & (1+\alpha) \\ (1+2\alpha) & (-\alpha-1) & (1-\alpha) & (1+\alpha) & (1+\alpha) \\ (1+2\alpha) & (-1-2\alpha) & 0 & (1+2\alpha) & 2\alpha \\ (1+2\alpha) & -1 & (1-\alpha) & (1+2\alpha) & (1+\alpha) \end{bmatrix}$$

$$\mathbf{Z}'\mathbf{Z} = \begin{bmatrix} 18(1+2\alpha)^2 & 0 & 0 & 0 & 0 \\ & 6(1-\alpha)^2 + 2(1+\alpha)^2 & & & 0 \\ & + 2(1+2\alpha)^2 + 2\alpha^2 + 2 & & & \\ & & 6(1-\alpha)^2 + 2(1+\alpha)^2 & & \\ & & + 2(1+2\alpha)^2 + 2\alpha^2 + 2 & & \\ & & & 12(1+2\alpha)^2 & \\ & & & 0 & \\ & & & 0 & \\ & & & 0 & \\ 8(1+\alpha)^2 + 14\alpha^2 & & & 4[(1+\alpha)^2 + \alpha(1+\alpha) & \\ + 4(1+2\alpha)^2 & & & + (1+2\alpha)(1+3\alpha) & \\ & & & 8(1+\alpha)^2 + 14\alpha^2 & \\ & & & + 4(1+2\alpha)^2 & \end{bmatrix} .$$

It may be noted that $|\mathbf{Z}'\mathbf{Z}| = 0$, if $\alpha = -0.5$.

For $\alpha = 0.1$,

$$\mathbf{Z}'\mathbf{Z} = \begin{bmatrix} 25.92 & 0 & 0 & 17.28 & 17.28 \\ 0 & 12.18 & 0 & 0 & 0 \\ 0 & 0 & 12.18 & 0 & 0 \\ 17.28 & 0 & 0 & 15.58 & 11.52 \\ 17.28 & 0 & 0 & 11.52 & 15.58 \end{bmatrix} ,$$

$$(\mathbf{Z}'\mathbf{Z})^{-1} = \begin{bmatrix} 0.2575 & 0 & 0 & -0.1642 & -0.1642 \\ 0 & 0.0821 & 0 & 0 & 0 \\ 0 & 0 & 0.0821 & 0 & 0 \\ -0.1642 & 0 & 0 & 0.2463 & 0 \\ -0.1642 & 0 & 0 & 0 & 0.2463 \end{bmatrix}.$$

Thus,

$$V(\hat{\beta}_0) = 0.2575\sigma^2, \quad V(\hat{\beta}_i) = 0.0821\sigma^2, \quad V(\hat{\beta}_{ii}) = 0.2463\sigma^2 \quad \text{and} \\ \text{Cov}(\hat{\beta}_0, \hat{\beta}_{ii}) = -0.1642\sigma^2, \quad i = 1, 2.$$

It can be seen that $V(\hat{y}) = 0.2575\sigma^2$ for all points in \mathbf{x} . Hence, the design is rotatable. It is interesting to note that for the class of designs presented here, $\text{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{i'i'}) = 0$. Hence, the quadratic effects are also estimated orthogonal to other effects except mean effect.

Figure 1 presents the variance of estimated response at different values of α varying from 0 to 1 for a second-order model ($v = 2, 3, 4$) with neighbor effects. It is seen that as the value of α increases, $\text{Var}(\hat{y})$ as well as the variance of parameter estimates decreases.

For negative values of α , as the value of α decreases, the variance of estimated response increases till $\alpha = -0.5$ (Fig. 2). At $\alpha = -0.5$, the matrix $\mathbf{Z}'\mathbf{Z}$ becomes singular and thus we do not get the variance. After $\alpha = -0.5$, the variance keeps on decreasing with the value of α until $\alpha = -1$.

It is thus concluded that incorporation of neighbor effects in the model influence the precision of predicted response and therefore should not be ignored.

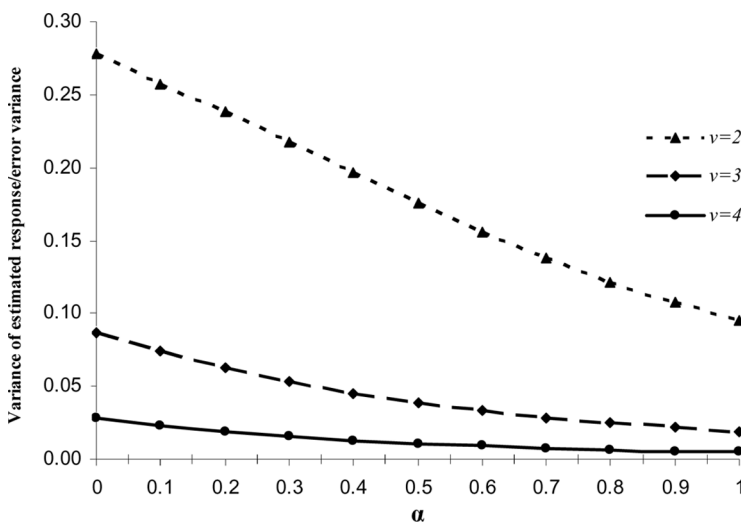


Figure 1. Relation between variance of estimated response and positive values of α .

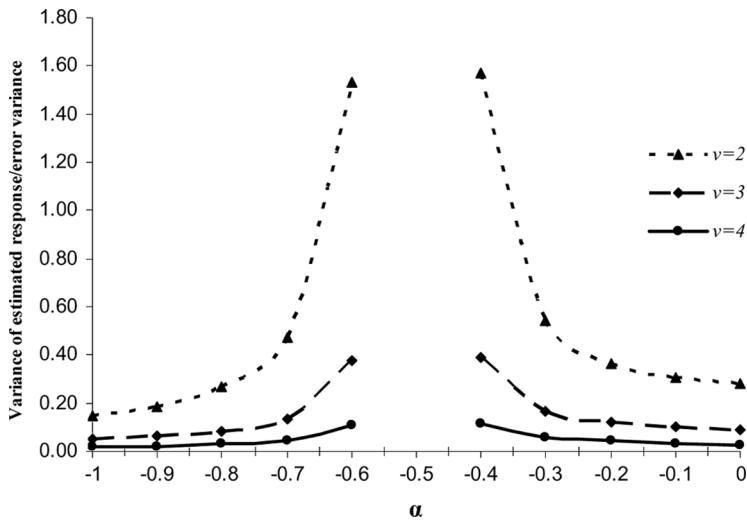


Figure 2. Relation between variance of estimated response and negative values of α .

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