FIRST ORDER ROTATABLE DESIGNS INCORPORATING NEIGHBOUR EFFECTS

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Abstract
In response surface analysis, it is generally assumed that the observations are independent and there is no effect of neighbouring units. But under the situation when the units are placed linearly with no gaps, the experimental units may experience neighbour or overlap effects from neighbouring units. Hence, for proper specification it is important to include the neighbour effects in the model. First order response surface model with neighbour effects from immediate left and right neighbouring units has been considered here and the conditions have been derived for the orthogonal estimation of coefficients of this model. The variance of estimated response has also been obtained and conditions for first order response surface model with neighbour effects to be rotatable have been obtained. A method of obtaining designs satisfying the derived conditions has been proposed. A first order rotatable design with neighbour effects using half replicate of 2^3 has also been given.

Keywords: Neighbour effects; orthogonal estimation; response surface; rotatable design.

1. Introduction

Response surface methodology explores the relationships between response variable(s) and several explanatory variables and the main idea is to obtain an optimal response using a set of designed points. The methodology includes setting up of an appropriately designed experiment, recording observations on the response of interest, determining 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.

Let there be v input factors (explanatory variables) $x_1, x_2, \ldots, x_v$ and a response variable y. The response is a function of input factors, i.e.,

$$y_u = f(x_{1u}, x_{2u}, x_{3u}, \ldots, x_{vu}) + e_u ; \; u = 1,2,\ldots,N \tag{1}$$

where x_{iu} is the level of the i^{th} factor $(i = 1,2,...,v)$ 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 the random error associated with the u^{th} observation which is assumed to be identically and independently distributed normally with mean zero and constant variance σ^2. f given in (1) is approximated, within the experimental region, by a polynomial of suitable degree in variables. Response surface models are polynomials which adequately represent the input-response relationship. The designs that allow the fitting of response surfaces and provide a measure for testing their adequacy are called response surface designs. For details on response surface methodology, one can refer to Box and Draper [2], Myers and Montgomery [6], Khuri and Cornell [1].

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 field experiments this assumption seems to be unrealistic. In field experiments, the neighbour effects from the treatments applied to the adjacent neighbouring plots may arise which may affect the response of the treatment applied to the plot under consideration. These neighbour effects are also called as overlap or interference or competition effects. For example, if one plot receives a spray chemical treatment, wind drift may cause the effect of spray spill over to 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 treatments combination 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 [5] suggested a general model for response surface problems in which it is anticipated that the response on a particular unit will be affected by overlap effects from neighbouring units and the same have been illustrated. Designs with neighbouring effects for single factor in block design setup have been extensively studied in the literature. (see e.g., Azais *et al.* [3], Tomar *et al.* [4] and Jaggi *et al.* [7]).

Here, we have studied the response surface model in which the experimental units experience the neighbour effects from immediate left and right neighbouring units assuming the units to be adjacent linearly with no gaps. Conditions have been derived for the orthogonal estimation of coefficients of first order response surface. Further, conditions for first order response surface model with neighbour effects to be rotatable have also been obtained. A method of constructing designs for fitting first order response surfaces in the presence of neighbour effects has also been developed and has been illustrated.

2. Response Surface Model with Neighbour Effects

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

$$y_u = f(x_u) + e_u \qquad u = 1,2,\ldots, N,$$

where $x_u = (x_{1u}, x_{2u}, \ldots, x_{vu})'$ defines the set of predictor values at which the response y_u is observed. The model incorporating the neighbour effects from immediate left and right neighbouring units can be written as:

$$y_u = \sum_{u \neq u'=1}^{N} g_{uu'} f(x_u) + e_u, \tag{2}$$

where

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

It may be mentioned here that the layout of the experiment for estimating this model includes border units for the end units. The treatment combinations applied on them are the treatment combinations from the experiment. Observations for border units are not modelled. Thus, model (2) can be written as

$$\mathbf{Y} = \mathbf{GX\beta} + \mathbf{e}, \tag{4}$$

where $\mathbf{G} = ((g_{uu'}))$ is the $N \times (N+2)$ neighbour matrix, $\mathbf{X}$ is a $(N+2) \times (v+1)$ matrix of N points (runs) with two border units (treatment combinations applied on these units are the treatment combinations from the N points) and v predictor variables with first column of unities, $\boldsymbol{\beta}$ is a $(v+1) \times 1$ vector of parameters and $\mathbf{e}$ is $N \times 1$ vector of errors which is $N(\mathbf{0}, \sigma^2\mathbf{I})$. If $\mathbf{G}$ is known, using Ordinary Least Squares (OLS) procedure, estimates of $\boldsymbol{\beta}$'s are obtained as follows in the presence of neighbour effects:

$$\hat{\boldsymbol{\beta}} = (\mathbf{Z'Z})^{-1}\mathbf{Z'Y}, \tag{5}$$

where

$$\mathbf{Z} = \mathbf{GX}$$

with

$$D(\hat{\boldsymbol{\beta}}) = \sigma^2 (\mathbf{Z'Z})^{-1}.$$

3. First Order Response Surface Model with Neighbour Effects

Let v = 2, the (N + 2) × 3 matrix **X** of 2 predictor variables with first column of 1's, the coefficients of mean and two extra points as border points is written as:

$$\mathbf{X}=\begin{bmatrix} 1 & x_{1N} & x_{2N} \\ \hline 1 & x_{11} & x_{21} \\ 1 & x_{12} & x_{22} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & x_{1u} & x_{2u} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & x_{1N} & x_{2N} \\ \hline 1 & x_{11} & x_{21} \end{bmatrix}$$

The N × (N + 2) neighbour matrix **G** as defined in (3) is

$$\mathbf{G}=\left[\begin{array}{c|cccccccc|c} \alpha & 1 & \alpha & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & \alpha & 1 & \alpha & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & \alpha & 1 & \alpha & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & \alpha & 1 & \alpha & . & . & . & 0 & 0 \\ . & . & . & . & & . & & & & . & . \\ . & . & . & . & & . & & & & . & . \\ . & . & . & . & & & & . & & . & . \\ 0 & 0 & 0 & 0 & . & . & . & \alpha & 1 & \alpha & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & \alpha & 1 & \alpha \end{array}\right] \tag{6}$$

Now,

$$\mathbf{Z}=\mathbf{GX}=\begin{bmatrix} (1+2\alpha) & x_{11}+\alpha(x_{1N}+x_{12}) & x_{21}+\alpha(x_{2N}+x_{22}) \\ (1+2\alpha) & x_{12}+\alpha(x_{11}+x_{13}) & x_{22}+\alpha(x_{21}+x_{23}) \\ (1+2\alpha) & x_{13}+\alpha(x_{12}+x_{14}) & x_{23}+\alpha(x_{22}+x_{24}) \\ . & . & . \\ . & . & . \\ . & . & . \\ (1+2\alpha) & x_{1u}+\alpha(x_{1(u-1)}+x_{1(u+1)}) & x_{2u}+\alpha(x_{2(u-1)}+x_{2(u+1)}) \\ . & . & . \\ . & . & . \\ . & . & . \\ (1+2\alpha) & x_{1N}+\alpha(x_{1(N-1)}+x_{11}) & x_{2N}+\alpha(x_{2(N-1)}+x_{21}) \end{bmatrix}$$

$$\mathbf{Z'Z} = \begin{bmatrix} N(1+2\alpha)^2 & (1+2\alpha)^2(\sum_{u=1}^{N} x_{1u}) & (1+2\alpha)^2(\sum_{u=1}^{N} x_{2u}) \\ . & (1+2\alpha^2)(\sum_{u=1}^{N} x_{1u}^2)+A_1 & (1+2\alpha^2)(\sum_{u=1}^{N} x_{1u}x_{2u})+C_{12} \\ & . & (1+2\alpha^2)(\sum_{u=1}^{N} x_{2u}^2)+A_2 \end{bmatrix} \tag{7}$$

where,

$$A_1 = 2\alpha^2\left[\sum_{u=1}^{N} x_{1u}x_{1[(u+2)\,\mathrm{mod}\,N]}\right] + 4\alpha\left[\sum_{u=1}^{N} x_{1u}x_{1[(u+1)\,\mathrm{mod}\,N]}\right]$$

$$A_2 = 2\alpha^2\left[\sum_{u=1}^{N} x_{2u}x_{2[(u+2)\,\mathrm{mod}\,N]}\right] + 4\alpha\left[\sum_{u=1}^{N} x_{2u}x_{2[(u+1)\,\mathrm{mod}\,N]}\right]$$

$$C_{12} = \alpha^2\left[\sum_{u=1}^{N} x_{1u}x_{2[(u+2)\,\mathrm{mod}\,N]} + \sum_{u=1}^{N} x_{1[(u+2)\,\mathrm{mod}\,N]}x_{2u}\right] + 2\alpha\left[\sum_{u=1}^{N} x_{1u}x_{2[(u+1)\,\mathrm{mod}\,N]} + \sum_{u=1}^{N} x_{1u}x_{2[(u-1)\,\mathrm{mod}\,N]}\right]$$

In general for v factors, the (N + 2) × (v + 1) matrix **X** with two extra points as border points is

$$\mathbf{X} = \left[\begin{array}{cccccccccc} 1 & x_{1N} & x_{2N} & . & . & . & x_{iN} & . & . & . & x_{vN} \\ \hline 1 & x_{11} & x_{21} & . & . & . & x_{i1} & . & . & . & x_{v1} \\ 1 & x_{12} & x_{22} & . & . & . & x_{i2} & . & . & . & x_{v2} \\ . & . & . & . & & & . & . & & & . \\ . & . & . & & . & & . & & . & & . \\ . & . & . & & & . & . & & & . & . \\ 1 & x_{1u} & x_{2u} & . & . & . & x_{iu} & . & . & . & x_{vu} \\ . & . & . & . & & & . & . & & & . \\ . & . & . & & . & & . & & . & & . \\ . & . & . & & & . & . & & & . & . \\ 1 & x_{1N} & x_{2N} & . & . & . & x_{iN} & . & . & . & x_{vN} \\ \hline 1 & x_{11} & x_{21} & . & . & . & x_{i1} & . & . & . & x_{v1} \end{array}\right]$$

The neighbour matrix **G** is of the form (6) which yields $\mathbf{Z'Z}$ as:

$$
\begin{bmatrix}
N(1+2\alpha)^2 & (1+2\alpha)^2\sum_{u=1}^{N}x_{1u} & (1+2\alpha)^2\sum_{u=1}^{N}x_{2u} & \cdots & (1+2\alpha)^2\sum_{u=1}^{N}x_{iu} & \cdots & (1+2\alpha)^2\sum_{u=1}^{N}x_{vu} \\
 & (1+2\alpha^2)\sum_{u=1}^{N}x_{1u}^2+A_1 & (1+2\alpha^2)\sum_{u=1}^{N}x_{1u}x_{2u}+C_{12} & \cdots & (1+2\alpha^2)\sum_{u=1}^{N}x_{1u}x_{iu}+C_{1i} & \cdots & (1+2\alpha^2)\sum_{u=1}^{N}x_{1u}x_{vu}+C_{1v} \\
 & & (1+2\alpha^2)\sum_{u=1}^{N}x_{2u}^2+A_2 & \cdots & (1+2\alpha^2)\sum_{u=1}^{N}x_{2u}x_{iu}+C_{2i} & \cdots & (1+2\alpha^2)\sum_{u=1}^{N}x_{2u}x_{vu}+C_{2v} \\
 & & & \ddots & \vdots & & \vdots \\
 & & & & (1+2\alpha^2)\sum_{u=1}^{N}x_{iu}^2+A_i & \cdots & (1+2\alpha^2)\sum_{u=1}^{N}x_{iu}x_{vu}+C_{iv} \\
 & & & & & \ddots & \vdots \\
 & & & & & & (1+2\alpha^2)\sum_{u=1}^{N}x_{vu}^2+A_v
\end{bmatrix} \tag{8}
$$

with $\alpha \neq -0.5$, otherwise $|\mathbf{Z'Z}| = 0$. Further,

$$
A_i = 2\alpha^2\left[\sum_{u=1}^{N} x_{iu}x_{i[(u+2)\bmod N]}\right] + 4\alpha\left[\sum_{u=1}^{N} x_{iu}x_{i[(u+1)\bmod N]}\right]
$$

$$
i = 1, 2, \ldots, v
$$

and

$$
C_{ii'} = \alpha^2\left[\sum_{u=1}^{N} x_{iu}x_{i'[(u+2)\bmod N]} + \sum_{u=1}^{N} x_{i[(u+2)\bmod N]}x_{i'u}\right] +
$$

$$
2\alpha\left[\sum_{u=1}^{N} x_{iu}x_{i'[(u+1)\bmod N]} + \sum_{u=1}^{N} x_{iu}x_{i'[(u-1)\bmod N]}\right]
$$

$$
i \neq i' = 1, 2, \ldots, v
$$

To ensure orthogonality in the estimation of the parameters, $\mathbf{Z'Z}$ has to be diagonal. This gives rise to the following conditions:

$$
\begin{aligned}
&\text{i)}\ \sum_{u=1}^{N} x_{iu} = 0 && \forall\ i = 1, 2, \ldots, v \\
&\text{ii)}\ \sum_{u=1}^{N} x_{iu}x_{i'u} = 0 && \forall\ i \neq i' = 1, 2, \ldots, v \\
&\text{iii)}\ C_{ii'} = 0 && \forall\ i \neq i' = 1, 2, \ldots, v
\end{aligned} \tag{9}
$$

Thus, in view of (9), $\mathbf{Z'Z}$ can be written as:

$$\begin{bmatrix} N(1+2\alpha)^2 & 0 & 0 & 0 & 0 \\ 0 & (1+2\alpha^2)\sum_{u=1}^{N}x_{1u}^2+A_1 & 0 & 0 & 0 \\ 0 & 0 & (1+2\alpha^2)\sum_{u=1}^{N}x_{2u}^2+A_2 & 0 & 0 \\ \vdots & & & & \vdots \\ 0 & 0 & 0 & (1+2\alpha^2)\sum_{u=1}^{N}x_{iu}^2+A_i & 0 \\ \vdots & & & & \vdots \\ 0 & 0 & 0 & 0 & (1+2\alpha^2)\sum_{u=1}^{N}x_{vu}^2+A_v \end{bmatrix} \qquad (10)$$

The normal equations for the estimation of (v +1) parameters are

$$\begin{bmatrix} N(1+2\alpha)^2 & \mathbf{0}' \\ \mathbf{0} & \mathbf{S} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \boldsymbol{\theta} \end{bmatrix} = \begin{bmatrix} Y. \\ \mathbf{T} \end{bmatrix}, \qquad (11)$$

where $\theta = (\beta_1\ \beta_2\ \beta_3\ \ldots\ \beta_v)'$ is the $v \times 1$ vector of parameters corresponding to predictor variables, $Y. = \sum_{u=1}^{N} y_u$ and $\mathbf{T} = (T_1, T_2, \ldots, T_i, \ldots, T_v)'$ is the vector of treatment combination totals, $T_i = \sum_{u=1}^{N} x_{iu} y_u$, $i = 1,2,\ldots,v$ and

$$S = \mathrm{diag}\left\{ \left[(1+2\alpha^2)\sum_{u=1}^{N} x_{1u}^2 + A_1\right] \ldots \left[(1+2\alpha^2)\sum_{u=1}^{N} x_{iu}^2 + A_i\right] \ldots \left[(1+2\alpha^2)\sum_{u=1}^{N} x_{vu}^2 + A_v\right] \right\}$$

Equation (11) yields

$$\begin{bmatrix} \hat{\beta}_0 \\ \hat{\boldsymbol{\theta}} \end{bmatrix} = \begin{bmatrix} N^{-1}(1+2\alpha)^{-2} Y. \\ S^{-1}\mathbf{T} \end{bmatrix} \qquad (12)$$

and

$$D\begin{bmatrix} \hat{\beta}_0 \\ \hat{\boldsymbol{\theta}} \end{bmatrix} = \sigma^2 \begin{bmatrix} N^{-1}(1+2\alpha)^{-2} & \mathbf{0}' \\ \mathbf{0} & S^{-1} \end{bmatrix}. \qquad (13)$$

We thus obtain the variance of parameter estimates as

$$V(\hat{\beta}_0) = \frac{\sigma^2}{N(1+2\alpha)^2}, \quad V(\hat{\beta}_i) = \frac{\sigma^2}{\left[(1+2\alpha^2)\sum_{u=1}^{N} x_{iu}^2 + A_i\right]}, \text{ for } i = 1,2,\ldots,v$$

The estimated response at the point x_0 is $\hat{y}_0 = x_0' \hat{\beta}$ with its variance

$$V(\hat{y}_0) = x_0' V(\hat{\beta}) x_0 = \sigma^2 x_0' (Z'Z)^{-1} x_0$$

Thus,

$$V(\hat{y}_0) = \sigma^2 \left\{ \begin{array}{l} \dfrac{1}{[N(1+2\alpha)^2]} + \dfrac{x_{10}^2}{\left[(1+2\alpha^2)\sum\limits_{u=1}^{N} x_{1u}^2 + A_1\right]} + \dfrac{x_{20}^2}{\left[(1+2\alpha^2)\sum\limits_{u=1}^{N} x_{2u}^2 + A_2\right]} \\ + \ldots + \dfrac{x_{i0}^2}{\left[(1+2\alpha^2)\sum\limits_{u=1}^{N} x_{iu}^2 + A_i\right]} + \ldots + \dfrac{x_{v0}^2}{\left[(1+2\alpha^2)\sum\limits_{u=1}^{N} x_{vu}^2 + A_v\right]} \end{array} \right\} \tag{14}$$

The constancy of the variances of the parameter estimates is ensured by the following conditions:

i) $\sum\limits_{u=1}^{N} x_{iu}^2 = \delta$, a constant $\forall\ i = 1, 2, \ldots, v$

ii) $A_i = A$, a constant $\forall\ i = 1, 2, \ldots, v$ (15)

Therefore,

$$V(\hat{y}_0) = \sigma^2 \left\{ \begin{array}{l} \dfrac{1}{N(1+2\alpha)^2} + \dfrac{x_{10}^2}{(1+2\alpha^2)\delta + A} + \ldots + \dfrac{x_{i0}^2}{(1+2\alpha^2)\delta + A} \\ \qquad + \ldots + \dfrac{x_{v0}^2}{(1+2\alpha^2)\delta + A} \end{array} \right\}$$

i.e.,

$$V(\hat{y}_0) = \sigma^2 \left\{ \dfrac{1}{N(1+2\alpha)^2} + \dfrac{\sum\limits_{i=1}^{v} x_{i0}^2}{(1+2\alpha^2)\delta + A} \right\}$$

Hence, the variances of β_i's (i =1,2,...,v) are same and it is seen that the variance of estimated response is a function of $\sum\limits_{i=1}^{v} x_{i0}^2$. For given α, the points for which $\sum\limits_{i=1}^{v} x_{i0}^2$ is same, the estimated response will have the same variance. The designs satisfying this property are called **First Order Rotatable Designs with Neighbour Effects (FORDNE)**. We now present a method of constructing FORDNE.

4. Method of Constructing FORDNE

Construct a 2^v full factorial for v factors each at 2 levels and arrange the combinations in lexicographic order in reverse order. Obtain $(v-1)2^v$ more combinations by circularly rotating the columns of 2^v factorial such that each column occupies all the v positions. The design so obtained is a FORDNE in $v \times 2^v$ points. Besides, two extra units are added as border units for neighbour effects.

Example 4.1: Let v = 2 with each factor at two levels, then we get four runs in full factorial. There are two columns for two factors. We write the second column below first column and first column below second column, i.e. first 2^2 runs are repeated with positions in each row shifted in circular fashion. Finally, we add the first run at the bottom and last run at the top as border rows. The 10 × 3 matrix **X** of 2 predictor variables with first column of 1's, the coefficients of mean and two extra points as border points and matrix **G** is written as follows:

$$\mathbf{X}=\begin{bmatrix} 1 & -1 & -1 \\ \hline 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ 1 & -1 & -1 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & -1 \\ \hline 1 & 1 & 1 \end{bmatrix}, \quad \mathbf{G}=\left[\begin{array}{c|cccccccc|c} \alpha & 1 & \alpha & 0 & 0 & 0 & . \; . \; . & 0 & 0 \\ 0 & \alpha & 1 & \alpha & 0 & 0 & . \; . \; . & 0 & 0 \\ 0 & 0 & \alpha & 1 & \alpha & 0 & . \; . \; . & 0 & 0 \\ 0 & 0 & 0 & \alpha & 1 & \alpha & . \; . \; . & 0 & 0 \\ . & . & . & . & & . & & . & . \\ . & . & . & . & & & . & . & . \\ . & . & . & . & & & . & . & . \\ 0 & 0 & 0 & 0 & . \; . \; . & \alpha & 1 & \alpha & 0 \\ 0 & 0 & 0 & 0 & . \; . \; . & 0 & \alpha & 1 & \alpha \end{array}\right],$$

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

and $$\mathbf{Z'}\,\mathbf{Z}=\begin{bmatrix} 8(1+2\alpha)^2 & 0 & 0 \\ 0 & 4+4(1-2\alpha)^2 & 0 \\ 0 & 0 & 4+4(1-2\alpha)^2 \end{bmatrix}$$ with $\alpha \neq -0.5$.

Therefore,

$$V(\hat{\beta}_0)=\frac{\sigma^2}{8(1+2\alpha)^2},\ V(\hat{\beta}_i)=\frac{\sigma^2}{4[1+(1-2\alpha)^2]}\ \text{for i =1,2 and}$$

$$V(\hat{y}_0)=\frac{\sigma^2}{8}\left\{\frac{1}{(1+2\alpha)^2}+\frac{2}{(1+2\alpha^2)-2\alpha}\right\}.$$

It can be seen that $V(\hat{\beta}_i)$ is maximum at $\alpha = 0.5$ for $v = 2$.
For $\alpha = 0.1$,

$$V(\hat{\beta}_0) = 0.0868\sigma^2,\ V(\hat{\beta}_i) = 0.1524\sigma^2,\ \text{i=1,2 and}\ V(\hat{y}_0) = 0.3916\sigma^2$$

Example 4.2: For v = 3 with each factor at two levels, the following design matrix of order 26×4 is obtained:

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

Further,

$$Z'Z=\begin{bmatrix} 24(1+2\alpha)^2 & 0'_{1\times 3} \\ 0_{3\times 1} & [4(1+2\alpha)^2+8(1-2\alpha)^2+12]\, I_3 \end{bmatrix},$$

Thus,

$$V(\hat{\beta}_0)=\frac{\sigma^2}{24(1+2\alpha)^2},$$

$$V(\hat{\beta}_i)=\frac{\sigma^2}{4[(1+2\alpha)^2+2(1-2\alpha)^2+3]} \quad i=1,2,3 \text{ and}$$

$$V(\hat{y}_0)=\frac{\sigma^2}{8}\left\{\frac{1}{3(1+2\alpha)^2}+\frac{3}{3(1+2\alpha^2)-2\alpha}\right\}$$

Here, the maximum of $V(\hat{\beta}_i)$ is attained at $\alpha = 0.16$.

For $\alpha = 0.4$,

$$V(\hat{\beta}_0)=0.0129\sigma^2,\ V(\hat{\beta}_i)=0.0396\sigma^2,\ i=1,2,3$$

and $V(\hat{y}_0)=0.1315\sigma^2$

Table 4.1 presents the variance of estimates at different values of α from 0 to 1 for v = 2, 3, 4, 5. It is seen that as the value of α increases, $\text{Var}(\hat{\beta}_0)$ decreases for all the values of α and v (= 2, 3, 4, 5). For v = 2, the $\text{Var}(\hat{\beta}_i)$ first increases as $\alpha \rightarrow 0.5$ and becomes maximum at $\alpha = 0.5$ and decreases there after till $\alpha = 1$ and exactly same is the case with Var($\hat{y}$). For v = 3, as indicated earlier, the $\text{Var}(\hat{\beta}_i)$ attains maximum at $\alpha = 0.16$, so it increases from $\alpha = 0$ till $\alpha = 0.2$ and there after, it keeps on decreasing till $\alpha = 1$; however, the Var($\hat{y}$) is not affected significantly, so it decreases as the value of α increases in the range 0 to 1. For v = 3, 4, the $\text{Var}(\hat{\beta}_i)$ and Var($\hat{y}$) both decrease with increase in the value of α from 0 to 1.

Figure 4.1 presents the variance of estimated response at different values of α varying from 0 to 1 for v = 2, 3, 4, 5. It is seen that as the value of α increases, $\text{Var}(\hat{y})$ decreases except for v = 2 with values of $\alpha \leq 0.8$.

Table 4.1: Variance of estimates at different values of α for first order model

v	$\frac{V(.)}{\sigma^2}$	α										
		0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
2	$\hat{\beta}_0$	0.1250	0.0868	0.0638	0.0488	0.0386	0.0313	0.0258	0.0217	0.0185	0.0159	0.0139
	$\hat{\beta}_i$	0.1250	0.1524	0.1838	0.2155	0.2404	0.2500	0.2404	0.2155	0.1838	0.1524	0.1250
	$\hat{y}$	0.3750	0.3916	0.4314	0.4798	0.5193	0.5313	0.5066	0.4527	0.3861	0.3208	0.2639
3	$\hat{\beta}_0$	0.0417	0.0289	0.0213	0.0163	0.0129	0.0104	0.0086	0.0072	0.0062	0.0053	0.0046
	$\hat{\beta}_i$	0.0417	0.0437	0.0440	0.0425	0.0396	0.0357	0.0316	0.0275	0.0239	0.0206	0.0179
	$\hat{y}$	0.1667	0.1601	0.1533	0.1438	0.1315	0.1176	0.1033	0.0898	0.0777	0.0672	0.0582
4	$\hat{\beta}_0$	0.0156	0.0109	0.0080	0.0061	0.0048	0.0039	0.0032	0.0027	0.0023	0.0020	0.0017
	$\hat{\beta}_i$	0.0156	0.0149	0.0137	0.0122	0.0107	0.0093	0.0080	0.0069	0.0059	0.0051	0.0045
	$\hat{y}$	0.0781	0.0705	0.0628	0.0550	0.0476	0.0409	0.0351	0.0302	0.0260	0.0225	0.0196
5	$\hat{\beta}_0$	0.0063	0.0043	0.0032	0.0024	0.0019	0.0016	0.0013	0.0011	0.0009	0.0008	0.0007
	$\hat{\beta}_i$	0.0063	0.0056	0.0049	0.0042	0.0036	0.0030	0.0026	0.0022	0.0019	0.0016	0.0014
	$\hat{y}$	0.0375	0.0324	0.0276	0.0233	0.0197	0.0166	0.0141	0.0120	0.0103	0.0089	0.0078

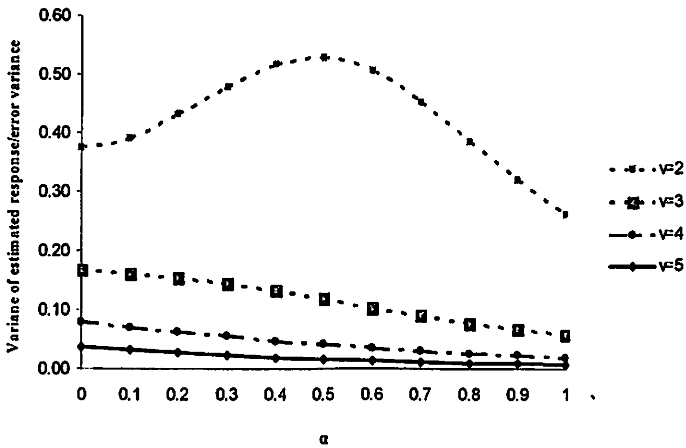

Fig. 4.1: Variance of estimated response for varying from 0 to 1

5. Another Design for Three Factors

Here, we present a FORDNE using a fraction of eight combinations resulting from three factors each at two levels. This is not a general method as described in Section 4.

Consider a half replicate of 2^3 resulting in 4 points in each replicate. Taking the non-key block, the three columns for three factors are circularly rotated resulting in 12 design points. Appropriately taking the border plots, the following design matrix is obtained:

$$\mathbf{X}=\left[\begin{array}{rrrr} 1 & 1 & 1 & 1 \\ \hline 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ \hline 1 & 1 & -1 & -1 \end{array}\right] \text{ and for } \alpha = 0.4,\ \mathbf{Z'Z}=\begin{bmatrix} 38.88 & 0 & 0 & 0 \\ 0 & 8.16 & 0 & 0 \\ 0 & 0 & 8.16 & 0 \\ 0 & 0 & 0 & 8.16 \end{bmatrix}$$

with $V(\hat{\beta}_0) = 0.0257\sigma^2$, $V(\hat{\beta}_i) = 0.1225\sigma^2, i = 1,2,3$ and $V(\hat{y}_0) = 0.3934$.

Table 5.1 presents the variance of estimates at different values of α from 0 to 1 for the above design. It is seen that as the value of α increases, $Var(\hat{\beta}_0)$ decreases, whereas $Var(\hat{\beta}_i)$ first increases till α = 0.5 and then decreases. Similar is the trend in case of $V(\hat{y})$. It is seen that the variance of estimates is almost doubled in case of taking a half fraction of 2^3 but there is saving with respect to the number of combinations required. Efficiency (Eff.) of this design as compared to full factorial with respect to variances of estimated response is also presented. The efficiency decreases as the value of α increases.

Concluding Remarks

It is seen that for two factors when $\alpha > 0.8$ and for three, four and five factors inclusion of neighbour effects in the model improves the precision of estimates of the parameters of the response model and results in more precise estimate of the predicted response at a given point. Hence, it is important to include the neighbour effects in the model to have the proper specification and to use a proper design.

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Table 5.1: Variance of estimates at different values of α for FORDNE obtained through a fraction of 2^3

$\frac{V(.)}{\sigma^2}$	α										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
$\hat{\beta}_0$	0.0833	0.0579	0.0425	0.0326	0.0257	0.0208	0.0172	0.0145	0.0123	0.0106	0.0093
$\hat{\beta}_i$	0.0833	0.0947	0.1059	0.1157	0.1225	0.1250	0.1225	0.1157	0.1059	0.0947	0.0833
$\hat{y}$	0.3333	0.3420	0.3603	0.3798	0.3934	0.3958	0.3849	0.3617	0.3301	0.2947	0.2593
Eff.	1.0003	0.9363	0.8510	0.7572	0.6685	0.5942	0.5368	0.4965	0.4708	0.4561	0.4489