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ROTATABLE RESPONSE SURFACE DESIGNS IN THE PRESENCE OF DIFFERENTIAL NEIGHBOUR EFFECTS FROM ADJOINING EXPERIMENTAL UNITS

ELDHO VARGHESE
SEEMA JAGGI
and
V. K. SHARMA
ICAR-Indian Agricultural Statistics Research Institute
New Delhi, India

ABSTRACT : In RSM, it is generally assumed that the observations are independent and there is no overlap effects from the neighbouring units. But in situations where the units are placed linearly side by side, there is a chance to have overlap effects/neighbour effects from the adjoining experiments units. For example, in field experiments if a chemical spray is applied to one plot, it may spread over to the nearby plots due to wind. Hence, the response from a particular plot may be affected by effects from the adjacent plots and this effect has to be included in the model while fitting RSM. In this paper, first and second order response surface models with differential effects from adjoining left and right neighbouring units has been considered and the conditions for the model with differential neighbour effects to be rotatable have been obtained. Method of obtaining designs satisfying the derived conditions has been described. An illustration to show the impact of including neighbour effects in the model on the parameter estimates has also been given using a simulated data set. These designs result in more precise estimates of the parameters of the response surface model.

Keywords and phrases : Response surface; Differential neighbour effects; Orthogonal estimation; FORDDNE; SORDDNE.

1. Introduction

Response Surface Methodology (RSM) consists of the experimental strategy for exploring relationship between the response variable and the input variables and to develop an appropriate relationship between them. It is used in situations where several input variables influence some performance measure or quality characteristic of a process. For details on response surface methodology, one can refer to Khuri and Cornell (1996), Montgomery and Peck (2006) and Myers et al. (2009).

The independence of observations cannot be ensured when experimental units are nearby without any separation. For example, in field experiments if a chemical fertilizer is applied to one plot, it may spread over to the nearby plots due to water seepage. Thus the response from a particular plot may also be affected by treatments applied to the adjacent plots and this effect of neighbouring plots has to be included in the model while fitting response surfaces. Hence, it is important to include the neighbour effects in the model to have the proper specification. The interdependence of plots are known in literature by different names viz., interference effects, neighbour effects, indirect effects, competition effect etc.

Indirect effects are effects which occur in an experiment due to the units which are adjacent (spatially or temporally) to the unit being observed. Spatial indirect effects arise due to the treatments applied to the adjacent neighbouring units/ plots and the designs so developed are called Neighbour Balanced Designs (NBDs) whereas temporal indirect effects occur because of the carryover or residual effects in the periods following the periods of their direct application and the designs considering temporal effects are called Crossover Designs. A large number of such designs have been developed in the literature. For details of NBDs, one can refer to Azais et al. (1993), Monod and Bailey (1993), Azais and Druilhet (1997), Azais et al. (1998), Bailey (2003), Bailey and Druilhet (2004), Tomar et al. (2005), Jaggi et al. (2006), Jaggi et al. (2007) and Pateria et al. (2007). For details of crossover designs, one can refer to Williams (1949), Patterson and Lucas (1962), Balaam (1968), Sharma (1975), Dey and Balachandran (1976), Sharma (1981), Sharma (1982), Afsarinejad (1990), Varghese and Sharma (2000), Sharma et al. (2002), Sharma et al. (2003) and Bose and Dey (2009). A software for the on line generation of such designs is available (Jaggi et al., 2015). Besides, incorporation of neighbour effects under two-way blocking setup is discussed by several authors [Freeman (1979), Federer and Basford (1991), Chan and Eccleston (2003), Varghese et al. (2011) and Varghese et al. (2014)].

The literature available on response surface designs incorporating neighbour effects is very few. Bartlett (1978) made an attempt to study the neighbouring plot-response relationships. 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 overlap effects from neighbouring units and the same have been illustrated.

Sarika et al. (2008) studied first order response surface model with equal neighbour effects 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. (2009) studied second order response surface model assuming equal neighbour effects and the expressions for the parameters were derived. A method of obtaining designs satisfying the derived conditions was given.

Jaggi et al. (2010) showed that if the neighbour effect is present and is included in the model, there is a substantial reduction in the residual sum of squares and the response is predicted more precisely. Therefore, it can be used to develop an appropriate approximating relationship between the response variable and the input variables when the experimental units are nearby and induce some neighbouring effects.

In response surface studies incorporating neighbour effects, it is unreasonable to expect the equal neighbour effects from adjacent plots always. Hence, we relax this condition of equality of neighbouring effects and present here response surface methodology considering differential effects from adjoining left and right neighbouring units and show that equality of variances as a particular case.

Consider the response surface model:

$$\boldsymbol{y}_u = f(\boldsymbol{X}_u) + \boldsymbol{e}_u \qquad u = 1, 2, \ldots, N,$$

where $\boldsymbol{y}_u$ is the response at the point u with input vector $\boldsymbol{X}_u = (X_{1u}, X_{2u}, \ldots, X_{vu})'$ of v components. We consider that the performance of a unit is influenced by the immediate left and immediate right units. Then, the model incorporating the differential neighbour effects from adjoining left and right neighbouring units can be written as:

$$y_{u'} = \sum_{u=1}^{N} g_{uu'} f(X_u) + e_{u'}, u' = 1, 2, \ldots, N \tag{1.1}$$

where

$$\left.\begin{aligned} g_{uu'} &= 1,\ \text{if } u = u' \\ &= \alpha_1, |\ \alpha_1\ | < 1,\ \text{if } u - u' = 1, u' < u \\ &= a_2, |\ \alpha_2\ | < 1,\ \text{if } u' - u = 1, u' > u \\ &= 0,\ \text{otherwise.} \end{aligned}\right\} \tag{1.2}$$

Here, α_1 represents left neighbour effect and α_2 represents the right neighbour effect. The layout of the experiment for estimating this model includes border units for the end units with $\boldsymbol{X}$ matrix given below at (2.1) and (3.2).

Direct effects of the border units are ignored. Thus, model (1.1) can be written as

$$\boldsymbol{Y} = \boldsymbol{G}\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{e}, \tag{1.3}$$

where $\boldsymbol{G} = ((g_{uu'}))$ is the $N \times (N+2)$ neighbour matrix. For a first order model, $\boldsymbol{X}$ is a $(N+2) \times (v+1)$ matrix of N points (runs) with two border units and v predictor variables with first column of unities, $\boldsymbol{\beta}$ is a $(v+1) \times 1$ vector of parameters and $\boldsymbol{e}$ is $N \times 1$ vector of errors which is $N(\boldsymbol{0}, \boldsymbol{\sigma}^2\boldsymbol{I})$. If $\boldsymbol{G}$ is known, the ordinary least squares (OLS) estimate of $\boldsymbol{\beta}$, in the presence of neighbour effects, is :

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{Z}'\boldsymbol{Z})^{-1}\boldsymbol{Z}'\boldsymbol{Y}, \tag{1.4}$$

where $\boldsymbol{Z} = \boldsymbol{GX}$ with $D(\hat{\boldsymbol{\beta}}) = \sigma^2(\boldsymbol{Z'Z})^{-1}$.
For example, when $v = 2$ and $N = 6$, then

$$\boldsymbol{X} = \left[\begin{array}{ccc} 1 & x_{16} & x_{26} \\ \hline 1 & x_{11} & x_{21} \\ 1 & x_{12} & x_{22} \\ 1 & x_{13} & x_{23} \\ 1 & x_{14} & x_{24} \\ 1 & x_{15} & x_{25} \\ 1 & x_{16} & x_{26} \\ \hline 1 & x_{11} & x_{21} \end{array}\right]$$

$$\boldsymbol{G} = \left[\begin{array}{c|cccccc|c} \alpha_1 & 1 & \alpha_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & \alpha_1 & 1 & \alpha_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha_1 & 1 & \alpha_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha_1 & 1 & \alpha_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & \alpha_1 & 1 & \alpha_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & \alpha_1 & 1 & \alpha_2 \end{array}\right]$$

$$\boldsymbol{GX} = \boldsymbol{Z} = \begin{bmatrix} (1+\alpha_1+\alpha_2) & x_{11}+\alpha_1 x_{16}+\alpha_2 x_{12} & x_{21}+\alpha_1 x_{26}+\alpha_2 x_{22} \\ (1+\alpha_1+\alpha_2) & x_{12}+\alpha_1 x_{11}+\alpha_2 x_{13} & x_{22}+\alpha_1 x_{21}+\alpha_2 x_{22} \\ (1+\alpha_1+\alpha_2) & x_{13}+\alpha_1 x_{12}+\alpha_2 x_{14} & x_{23}+\alpha_1 x_{22}+\alpha_2 x_{24} \\ (1+\alpha_1+\alpha_2) & x_{14}+\alpha_1 x_{13}+\alpha_2 x_{15} & x_{24}+\alpha_1 x_{23}+\alpha_2 x_{25} \\ (1+\alpha_1+\alpha_2) & x_{15}+\alpha_1 x_{14}+\alpha_2 x_{16} & x_{25}+\alpha_1 x_{24}+\alpha_2 x_{26} \\ (1+\alpha_1+\alpha_2) & x_{16}+\alpha_1 x_{15}+\alpha_2 x_{11} & x_{26}+\alpha_1 x_{25}+\alpha_2 x_{21} \end{bmatrix}$$

Note : If α_1 and α_2 are known, $\hat{\beta}_i$'s are best linear unbiased estimates for β_i's. However, the values of α_1 and α_2 are hardly known in practice. In that case, one of the procedures, that has been adopted here, is to estimate β_i's by scanning the entire range of $\alpha_1, \alpha_2 \in \{0, 1\}$ and choose the values for which the residual sum of squares is minimum. The estimates are still supposed to have their asymptotic properties.

2. First Order Response Surface Model with Differential Neighbour Effects

Here, the function $f(x_u)$ takes the form $f(x_u) = \beta_0 + \sum_{i=1}^{v} \beta_i x_{iu}$. The response surface model for $v = 2$ incorporating indirect effect can be expressed as
$y_u = (1+\alpha_i+\alpha_2)\beta_0 + \beta_1(x_{1u} + \alpha_1 x_{1,u-1} + \alpha_2 x_{1,u+1}) + \beta_2(x_{2u} + \alpha_1 x_{2,u-1} + \alpha_2 x_{2,u+1}) + \varepsilon_u$, where $u = 1, 2, \ldots, N, u = 0$ for left most border plot and $u = N + 1$ for right most border plot.

In matrix notation, for v factors, the $(N+2)\times(v+1)$ matrix $\boldsymbol{X}$ with two extra points as border points is

$$\boldsymbol{X} = \left[\begin{array}{cccccccccccc}
1 & x_{1N} & x_{2N} & . & . & . & x_{iN} & . & . & . & x_{vN} \\ \hline
1 & x_{11} & x_{21} & . & . & . & x_{i1} & . & . & . & x_{v1} \\
1 & x_{12} & x_{22} & . & . & . & x_{i2} & . & . & . & x_{v2} \\
. & . & . & . & & & . & . & & & . \\
. & . & . & & . & & . & & . & & . \\
. & . & . & & & . & . & & & . & . \\
1 & x_{1u} & x_{2u} & . & . & . & x_{iu} & . & . & . & x_{vu} \\
. & . & . & . & & & . & . & & & . \\
. & . & . & & . & & . & & . & & . \\
. & . & . & & & . & . & & & . & . \\
1 & x_{1N} & x_{2N} & . & . & . & x_{iN} & . & . & . & x_{vN} \\ \hline
1 & x_{11} & x_{21} & . & . & . & x_{i1} & . & . & . & x_{v1}
\end{array}\right] \tag{2.1}$$

The neighbour matrix $\boldsymbol{G}$ is of the form (1.2) which yields $\boldsymbol{Z'Z}$ as:

$$\begin{bmatrix}
pN & p\sum_{u=1}^{N} X_{1u} & p\sum_{u=1}^{N} X_{2u} & \dots & p\sum_{u=1}^{N} X_{iu} & \dots & p\sum_{u=1}^{N} X_{vu} \\
 & q\sum_{u=1}^{N} X_{1u}^2 + A_1 & q\sum_{u=1}^{N} X_{1u}X_{2u} & \dots & q\sum_{u=1}^{N} X_{1u}X_{iu} + C_{1i} & \dots & q\sum_{u=1}^{N} X_{1u}X_{vu} + C_{1v} \\
 & & q\sum_{u=1}^{N} X_{2u}^2 + A_2 & \dots & q\sum_{u=1}^{N} X_{2u}X_{iu} + C_{2i} & \dots & q\sum_{u=1}^{N} X_{2u}X_{vu} + C_{2v} \\
 & & & \vdots & & & \\
 & & & & q\sum_{u=1}^{N} X_{1u}^2 + A_i & \dots & q\sum_{u=1}^{N} X_{iu}X_{vu} + C_{iv} \\
 & & & \vdots & & & \\
 & & & & & & q\sum_{u=1}^{N} X_{vu}^2 + A_v
\end{bmatrix} \tag{2.2}$$

where $p=(1+\alpha_1+\alpha_2)^2$ and $q=(1+\alpha_1^2+\alpha_2^2)$, with $\alpha_1+\alpha_2 \neq -1$, otherwise $\mid \boldsymbol{Z'Z} \mid = 0$. Further,

$$A_i = 2\alpha_1\alpha_2\left[\sum_{u=1}^{N} X_{iu}X_{i[(u+2)\bmod N]}\right] + 2(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{iu}X_{i[(u+1)\bmod N]}\right]$$
$$i = 1, 2, \dots, v;$$

and

$$C_{ii'} = \alpha_1\alpha_2\left[\sum_{u=1}^{N} X_{iu}X_{i'[(u+2)\bmod N]} + \sum_{u=1}^{N} X_{i[(u+2)\bmod N]}X_{i'u}\right] +$$

$$(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{iu}X_{i'[(u+1)\,\mathrm{mod}N]}\right]+\sum_{u=1}^{N} X_{iu}X_{i'[(u-1)\,\mathrm{mod}N]}\Bigg]$$
$$\forall\ i\neq i'=1,2,\ldots,v.$$

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

$$\begin{aligned}
&\text{i) } \sum_{u=1}^{N} X_{iu}=0 && \forall\ i=1,2,\ldots,v;\\
&\text{ii) } \sum_{u=1}^{N} X_{iu}X_{i'u}=0 && \forall\ i\neq i'=1,2,\ldots,v;\\
&\text{iii) } C_{ii'}=0 && \forall\ i\neq i'=1,2,\ldots,v.
\end{aligned} \tag{2.3}$$

After imposing the restrictions, the normal equations for the estimation of $(v+1)$ parameters are

$$\begin{bmatrix} N(1+\alpha_1+\alpha_2)^2 & \boldsymbol{0'}\\ \boldsymbol{0} & \boldsymbol{S}\end{bmatrix}\begin{bmatrix}\beta_0\\ \boldsymbol{\theta}\end{bmatrix}=\begin{bmatrix} Y.\\ \boldsymbol{T}\end{bmatrix}, \tag{2.4}$$

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

$$\boldsymbol{S}=\ \text{diag}\ \left\{\left[(1+\alpha_1^2+\alpha_2^2)\sum_{u=1}^{N} X_{1u}^2+A_1\right]\cdots\right.$$
$$\left.\left[(1+\alpha_1^2+\alpha_2^2)\sum_{u=1}^{N} X_{1u}^2+A_i\right]\cdots\left[(1+\alpha_1^2+\alpha_2^2)\sum_{u=1}^{N} X_{vu}^2+A_v\right]\right\}$$

Equation (2.4) gives

$$\begin{bmatrix}\hat\beta_0\\ \hat{\boldsymbol{\theta}}\end{bmatrix}=\begin{bmatrix} N^{-1}(1+\alpha_1+\alpha_2)^{-2}Y.\\ \boldsymbol{S^{-1}T}\end{bmatrix} \tag{2.5}$$

Hence, the variance of parameter estimates is obtained as

$$\begin{aligned}
V(\hat\beta_0) &= \frac{\sigma^2}{N(1+\alpha_1+\alpha_2)^2};\\
V(\hat\beta_i) &= \frac{\sigma^2}{\left[(1+\alpha_1^2+\alpha_2^2)\sum_{u=1}^{N} X_{iu}^2+A_i\right]},\ \text{for } i=1,2,\ldots,v.
\end{aligned}$$

The estimated response at a point, say $\boldsymbol{x}_0$ is $\hat y_0=\boldsymbol{x'}_0\hat{\boldsymbol{\beta}}$ with variance

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

Thus,

$$V(\hat{y}_0) =$$

$$\sigma^2 \left\{ \begin{array}{c} \frac{1}{[N(1+\alpha_1+\alpha_2)^2]} + \frac{x_{10}^2}{\left[(1+\alpha_1^2+\alpha_2^2)\sum\limits_{u=1}^{N} X_{1u}^2 + A_1\right]} + \frac{x_{20}^2}{\left[(1+\alpha_1^2+\alpha_2^2)\sum\limits_{u=1}^{N} X_{2u}^2 + A_2\right]} \\ + \ldots + \frac{x_{i0}^2}{\left[(1+\alpha_1^2+\alpha_2^2)\sum\limits_{u=1}^{N} X_{1u}^2 + A_i\right]} + \ldots + \frac{x_{v0}^2}{\left[(1+\alpha_1^2+\alpha_2^2)\sum\limits_{u=1}^{N} X_{vu}^2 + A_v\right]} \end{array} \right\} \tag{2.6}$$

Now, the following restrictions are imposed to ensure the constancy of the variances of the parameter estimates

$$\begin{array}{l} \text{i) } \sum\limits_{u=1}^{N} X_{iu}^2 = \delta, \text{a constant } \forall\ i = 1, 2, \ldots, v \\ \text{ii) } A_i = A, \text{ a constant } \forall\ i \neq i' = 1, 2, \ldots, v \end{array} \tag{2.7}$$

Therefore,

$$V(\hat{y}_0) = \sigma^2 \left\{ \frac{1}{N(1+\alpha_1+\alpha_2)^2} + \frac{\sum\limits_{u=1}^{N} X_{i0}^2}{(1+\alpha_1^2+\alpha_2^2)\delta + A} \right\}$$

Hence, the variances of $\hat{\beta}_i$'s $(i = 1, 2, \ldots, v)$ 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_1 and α_2, 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 Differential Neighbour Effects (FORDDNE).

Remark 2.1 For $\alpha_1 = \alpha_2 = \alpha$, the above expressions reduce to those given in Sarika *et al.* (2008).

2.1 Method of Constructing FORDDNE

Construct a 2^v full factorial in lexicographic order with levels $(-1, 1)$ giving a rectangle R of 2^v rows and v columns with entries -1 and 1. Circular rotation of the columns of $R, (v-1)$ times, yields $(v-1)$ sets each consisting of 2^v rows and v columns. By appending these sets below R one after another, we obtain a rectangular array of $v \times 2^v$ rows and v columns. Appending another column of unity resulting in $(v+1)$ columns, a FORDDNE in $v \times 2^v$ points is obtained by adding two extra points of border units such that each end of the array has a point of the other end.

Example 2.1 Let $v = 3$. The 24×4 of a FORDDNE developed from a complete 2^3 factorial with levels -1 and 1 by rotating its columns 2 times with first column of 1's, the coefficient of mean, and two extra points as border points is written as follows:

$$\left[\begin{array}{rrrr}
1 & -1 & -1 & -1 \\
\hline
1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 \\
1 & 1 & -1 & 1 \\
1 & 1 & -1 & -1 \\
1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 \\
1 & -1 & -1 & -1 \\
1 & 1 & 1 & 1 \\
1 & -1 & 1 & 1 \\
1 & 1 & 1 & -1 \\
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1 & 1 & -1 & -1 \\
1 & -1 & -1 & -1 \\
1 & 1 & 1 & 1 \\
1 & 1 & -1 & 1 \\
1 & -1 & 1 & 1 \\
1 & -1 & -1 & 1 \\
1 & 1 & 1 & -1 \\
1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1 \\
1 & -1 & -1 & -1 \\
\hline
1 & 1 & 1 & 1
\end{array}\right]$$

The matrix $\boldsymbol{G}$ of order 27×29 is of the form given in (1.2). Further.

$$\boldsymbol{Z}'\boldsymbol{Z} = \begin{bmatrix} 24(1+\alpha_1+\alpha_2)^2 & \mathbf{0'}_{1\times 3} \\ \mathbf{0}_{3\times 1} & [4(1+\alpha_1+\alpha_2)^2 + 8(1-\alpha_1-\alpha_2)^2 + 12]\boldsymbol{I}_3 \end{bmatrix},$$

with $\alpha_1 = \alpha_2 \neq -0.5$
Thus,

$$V(\hat{\beta}_0) = \frac{\sigma^2}{24(1+\alpha_1+\alpha_2)^2},$$

$$V(\hat{\beta}_i) = \frac{\sigma^2}{[4(1+\alpha_1+\alpha_2) + 8(1-\alpha_1-\alpha_2)^2 + 12]}, i = 1, 2, 3$$

$$V(\hat{y}_0) = \sigma^2 \left\{ \frac{1}{24(1+\alpha_1+\alpha_2)^2} + \frac{3}{12(\alpha_1+\alpha_2)^2 - 8(1-\alpha_1-\alpha_2)^2 + 24} \right\}$$

For $\alpha_1 = 0.2$ and $\alpha_2 = 0.4$,

$$V(\hat{\beta}_0) = 0.0163\sigma^2, V(\hat{\beta}_i) = 0.0425\sigma^2, i = 1,2,3 \text{ and } V(\hat{y}_0) = 0.1438\sigma^2$$

2.2 Illustration

For the design given in Example 2.1, following is the synthetic data with plot numbers and treatment combinations:

Border plot	Plot 1	Plot 2	Plot 3	Plot 4	Plot 5
(1-1-1-1)	(1111)	(111-1)	(11-11)	(11-1-1)	(1-111)
	144.06	158.62	164.87	162.01	131.16

Plot 6	Plot 7	Plot 8	Plot 9	Plot 10	Plot 11	Plot 12
(1-11-1)	(1-1-11)	(1-1-1-1)	(1111)	(1-111)	(111-1)	(1-11-1)
116.94	123.25	137.26	140.68	141.06	125.73	131.61

Plot 13	Plot 14	Plot 15	Plot 16	Plot 17	Plot 18	Plot 19
(11-11)	(11-1-1)	(1-1-11)	(11-1-1)	(1111)	(11-11)	(1-111)
146.75	161.87	146.77	143.93	153.43	164.85	148.95

Plot 20	Plot 21	Plot 22	Plot 23	Plot 24	Border plot
(1-1-11)	(111-1)	(11-11-1)	(11-1-1)	(1-1-1-1)	(1111)
135.75	146.41	141.25	125.13	122.35	

Here, plot 1 has border plot as left neighbouring plot and plot 2 as right neighbouring plot, plot 2 has plot 1 as left neighbouring plot and plot 3 as right neighbouring plot and so on. First order response surface model was fitted to these data with three factors. The coefficient of determination (R^2), Residual Sum of Squares (RSS) and the parameter estimates for different values of α_1 and α_2 were calculated and are given in Table 2.1. It can be seen that RSS is 2556.45 at $\alpha_1 = 0$ and $\alpha_2 = 0$ which decreases as the value of α_1 and α_2 increases and is minimum at $\alpha_1 = 0.78$ and $\alpha_2 = 0.47$. Similar trend can be seen for $R^2 = 99.98\%$ at $\alpha_1 = 0.78$ and $\alpha_2 = 0.47$. All the parameters except β_0 and β_1 are not significant at $\alpha_1 = \alpha_2 = 0$ where as all the parameters become significant at $\alpha_1 = 0.78$ and $\alpha_2 = 0.47$ clearly indicating the impact of the neighbouring units. The fitted model at $\hat{\alpha}_1 = 0.78$ and $\hat{\alpha}_2 = 0.47$ is:

$$\hat{y} = 63.24 + 9.26X_1 - 4.63X_2 + 5.25X_3$$

The variance of the estimated responses is same for all the points within the design and is obtained as 0.097 at $\alpha_1 = 0.78$ and $\alpha_2 = 0.47$. Hence the design is rotatable. The maximum response corresponds to the maximum dose of the input factors X_1 and X_3 and minimum dose of the input factor X_2. The variance of the estimated response for all the points within the design at $\alpha_1 = \alpha_2 = 0$ is worked out as 0.170.

Table 2.1 Results of fitting first order model for $v = 3$ at different values of α_1 and α_2

α_2	α_1	**0.00**	**0.20**	**0.40**	**0.60**	**0.70**	**0.75**	**0.78**	**0.80**	**0.90**
0.00	R^2	0.4480	0.6046	0.7379	0.8172	0.8364	0.8417	0.8436	0.8444	0.8433
	RSS	2556.45	1807.39	1198.26	835.79	747.84	723.86	715.13	711.49	716.24
	$\hat{\beta}_0$	142.28* (2.31)	118.56* (1.62)	101.63* (1.13)	88.92* (0.82)	83.69* (0.73)	81.30* (0.70)	79.93* (0.69)	79.04* (0.68)	74.88* (0.64)
	$\hat{\beta}_1$	7.34* (2.31)	8.71* (1.97)	9.36* (1.56)	9.26*2 (0.23)	8.99* (1.11)	8.83* (1.07)	8.72* (1.05)	8.64* (1.04)	8.24* (0.99)
	$\hat{\beta}_2$	-3.63 (2.31)	-4.32 (1.97)	-4.65* (1.56)	-4.61* (1.23)	-4.48* (1.11)	-4.40* (1.07)	-4.35* (1.05)	-4.31* (1.04)	-4.11* (0.99)
	$\hat{\beta}_3$	4.11 (2.31)	4.89 (1.97)	5.27* (1.56)	5.22* (1.23)	5.08* (1.11)	4.98* (1.07)	4.92* (1.05)	4.88* (1.04)	4.65* (0.99)
0.20	R^2	0.5264	0.7086	0.8506	0.9279	0.9432	0.9460	0.9464	0.9461	0.9392
	RSS	2165.03	1332.10	683.10	329.50	259.52	246.73	245.22	246.57	277.73
	$\hat{\beta}_0$	118.57* (1.77)	101.63* (1.19)	88.92* (0.75)	79.04* (0.46)	74.88* (0.39)	72.96* (0.37)	71.86* (0.36)	71.14* (0.36)	67.75* (0.36)
	$\hat{\beta}_1$	8.12* (2.15)	9.55* (1.71)	10.17* (1.19)	9.97*2 (0.78)	9.65* (0.66)	9.45* (0.63)	9.32* (0.62)	9.23* (0.62)	8.77* (0.62)
	$\hat{\beta}_2$	-4.03 (2.15)	-4.74* (1.71)	-5.06* (1.19)	-4.97* (0.78)	-4.81* (0.66)	-4.71* (0.63)	-4.65* (0.62)	-4.61* (0.62)	-4.38* (0.62)
	$\hat{\beta}_3$	4.57 (2.15)	5.38 (1.71)	5.74* (1.19)	5.64* (0.78)	5.46* (0.66)	4.35* (0.63)	5.27* (0.62)	5.23* (0.62)	4.96* (0.62)
0.40	R^2	0.5740	0.7585	0.9009	0.9782	0.9932	0.9958	0.9960	0.9956	0.9881
	RSS	1947.32	1104.03	452.94	99.82	30.97	19.07	18.22	20.06	54.35
	$\hat{\beta}_0$	101.63* (1.44)	88.92* (0.89)	79.04* (0.54)	71.14* (0.23)	67.75* (0.12)	66.18* (0.09)	65.27* (0.13)	64.67* (0.09)	61.86* (0.14)
	$\hat{\beta}_1$	8.25* (1.99)	9.60* (1.47)	10.19* (0.95)	10.00* (0.42)	9.69* (0.22)	9.50* (0.17)	9.37* (0.23)	9.29* (0.17)	8.83* (0.27)
	$\hat{\beta}_2$	-4.10 (1.99)	-4.78* (1.47)	-5.08* (0.95)	-4.99* (0.42)	-4.84* (0.22)	-4.74* (0.17)	-4.68* (0.23)	-4.64* (0.17)	-4.41* (0.27)
	$\hat{\beta}_3$	4.65 (1.99)	5.43* (1.47)	5.77* (0.95)	5.66* (0.42)	5.49* (0.22)	5.38* (0.17)	5.31* (0.23)	5.26* (0.17)	5.01* (0.27)
0.45	R^2	0.5790	0.7616	0.029	0.9805	0.9961	0.9991	0.9994	0.9992	0.9923
	RSS	1924.50	1089.52	443.76	89.08	17.70	4.32	2.56	3.79	35.01
	$\hat{\beta}_0$	98.12* (1.38)	86.23* (0.91)	76.91* (0.52)	69.40* (0.21)	66.18* (0.09)	64.67* (0.04)	63.80* (0.03)	63.24* (0.03)	60.54* (0.11)
	$\hat{\beta}_1$	8.18* (1.95)	9.50* (1.49)	10.08* (0.93)	9.90* (0.39)	9.61* (0.17)	9.42* (0.08)	9.30* (0.06)	9.22* (0.07)	8.77* (0.22)
	$\hat{\beta}_2$	-4.06 (1.95)	-4.73* (1.49)	-5.02* (0.93)	-4.94* (0.39)	-4.80* (0.17)	-4.70* (0.08)	-4.65* (0.06)	-4.60* (0.07)	-4.38* (0.22)
	$\hat{\beta}_3$	4.62 (1.95)	5.37* (1.49)	5.71* (0.93)	5.61* (0.39)	5.45* (0.17)	5.34* (0.08)	5.27* (0.06)	5.23* (0.07)	4.98* (0.22)

	R^2	0.5803	0.7618	0.9026	0.9804	0.9963	0.9994	0.9998	0.9997	0.9932
	RSS	1918.77	1088.76	445.12	89.69	17.04	2.92	0.69	1.59	31.22
	$\hat{\beta}_0$	96.79*	85.20*	76.08*	68.73*	65.57*	64.09*	63.24*	62.68*	60.03*
		(1.36)	(0.90)	(0.51)	(0.21)	(0.09)	(0.04)	(0.02)	(0.03)	(0.11)
0.47	$\hat{\beta}_1$	8.14*	9.45*	10.02*	9.86*	9.56*	9.38*	9.26*	9.18*	8.74*
		(1.93)	(1.48)	(0.92)	(0.39)	(0.16)	(0.07)	(0.03)	(0.03)	(0.20)
	$\hat{\beta}_2$	-4.05	-4.70*	-4.99*	-4.92*	-4.78*	-4.69*	-4.63*	-4.59*	-4.37*
		(1.93)	(1.48)	(0.92)	(0.39)	(0.16)	(0.07)	(0.03)	(0.05)	(0.20)
	$\hat{\beta}_3$	4.60	5.34*	5.68*	5.59*	5.42*	5.32*	5.25*	5.21*	4.96*
		(1.93)	(1.48)	(0.92)	(0.39)	(0.16)	(0.07)	(0.03)	(0.05)	(0.20)
	R^2	0.5814	0.7612	0.9011	0.9791	0.9954	0.9988	0.9994	0.9994	0.9935
	RSS	1913.67	1091.58	452.26	95.61	20.84	5.44	2.40	2.77	29.63
	$\hat{\beta}_0$	94.85*	83.69*	74.88*	67.75*	64.67*	63.24*	62.40*	61.86*	59.28*
		(1.33)	(0.89)	(0.51)	(0.21)	(0.09)	(0.05)	(0.03)	(0.03)	(0.10)
0.50	$\hat{\beta}_1$	8.08*	9.35*	9.93*	9.77*	9.49*	9.31*	9.20*	9.12*	8.69*
		(1.92)	(1.47)	(0.92)	(0.40)	(0.18)	(0.09)	(0.06)	(0.06)	(0.20)
	$\hat{\beta}_2$	-4.01	-4.66*	-4.95*	-4.88*	-4.74*	-4.65*	-4.60*	-4.56*	-4.34*
		(1.92)	(1.47)	(0.92)	(0.40)	(0.18)	(0.09)	(0.06)	(0.06)	(0.20)
	$\hat{\beta}_3$	4.57	5.29*	5.62*	5.54*	5.38*	5.28*	5.22*	5.17*	4.93*
		(1.92)	(1.47)	(0.92)	(0.40)	(0.18)	(0.09)	(0.06)	(0.06)	(0.20)
	R^2	0.5791	0.7514	0.8871	0.9661	0.9843	0.9889	0.9903	0.9907	0.9874
	RSS	1924.40	1136.56	515.90	154.98	71.56	50.88	44.49	42.55	57.59
	$\hat{\beta}_0$	88.92*	79.04*	71.14*	64.67*	61.86*	60.54*	59.78*	59.28*	56.91*
		(1.25)	(0.85)	(0.52)	(0.26)	(0.17)	(0.14)	(0.13)	(0.12)	(0.14)
0.60	$\hat{\beta}_1$	7.79*	8.97*	9.52*	9.42*	9.18*	9.02*	8.92*	8.85*	8.46*
		(1.86)	(1.45)	(0.95)	(0.49)	(0.32)	(0.27)	(0.23)	(0.24)	(0.27)
	$\hat{\beta}_2$	-3.87	-4.47*	-4.75*	-4.70*	-4.58*	-4.51*	-4.46*	-4.42*	-4.23*
		(1.86)	(1.45)	(0.95)	(0.49)	(0.32)	(0.27)	(0.23)	(0.24)	(0.27)
	$\hat{\beta}_3$	4.41	5.08*	5.40*	5.35*	5.21*	5.12*	5.06*	5.02*	4.81*
		(1.86)	(1.45)	(0.95)	(0.49)	(0.32)	(0.27)	(0.23)	(0.24)	(0.27)
	R^2	0.5530	0.7055	0.8299	0.9099	0.9323	0.9396	0.9428	0.9445	0.9477
	RSS	2043.54	1346.50	777.43	412.05	309.27	276.08	261.51	253.91	238.91
	$\hat{\beta}_0$	79.04*	71.14*	64.67*	59.28*	56.91*	55.80*	55.15*	54.72*	52.70*
		(1.47)	(0.84)	(0.58)	(0.39)	(0.32)	(0.30)	(0.29)	(0.28)	(0.26)
0.80	$\hat{\beta}_1$	6.98*	7.97*	8.47*	8.48*	8.32*	8.21*	8.14*	8.09*	7.80*
		(1.76)	(1.44)	(1.08)	(0.75)	(0.63)	(0.58)	(0.56)	(0.55)	(0.51)
	$\hat{\beta}_2$	-3.48	-3.97*	-4.23*	-4.24*	-4.16*	-4.11*	-4.07*	-4.05*	-3.90*
		(1.76)	(1.44)	(1.08)	(0.75)	(0.63)	(0.58)	(0.56)	(0.55)	(0.51)
	$\hat{\beta}_3$	3.97	4.53	4.82*	4.82*	4.73*	4.67*	4.63*	4.60*	4.44*
		(1.76)	(1.44)	(1.08)	(0.75)	(0.63)	(0.58)	(0.56)	(0.55)	(0.51)
	R^2	0.5333	0.6750	0.7930	0.8725	0.8968	0.9054	0.9094	0.9117	0.9183
	RSS	2133.42	1485.71	946.48	582.84	471.74	432.69	414.20	403.82	373.64
	$\hat{\beta}_0$	74.88*	67.75*	61.86*	56.91*	54.72*	53.69*	53.10*	52.70*	50.82*
		(1.11)	(0.84)	(0.61)	(0.44)	(0.38)	(0.36)	(0.35)	(0.34)	(0.32)
0.90	$\hat{\beta}_1$	6.54*	7.43*	7.90*	7.96*	7.84*	7.75*	7.69*	7.65*	7.42*
		(1.72)	(1.44)	(1.13)	(0.85)	(0.75)	(0.70)	(0.68)	(0.67)	(0.62)
	$\hat{\beta}_2$	-3.26	-3.71*	-3.95*	-3.98*	-3.92*	-3.88*	-3.85*	-3.83*	-3.71*
		(1.72)	(1.44)	(1.13)	(0.85)	(0.75)	(0.70)	(0.68)	(0.67)	(0.62)
	$\hat{\beta}_3$	3.72	4.22	4.50*	4.53*	4.46*	4.41*	4.38*	4.36*	4.22*
		(1.72)	(1.44)	(1.13)	(0.85)	(0.75)	(0.70)	(0.68)	(0.67)	(0.62)

Figures within parentheses are the standard errors of the estimates $*p < 0.01$

Even though the method explained above gives designs which ensure the constancy in variance of the estimated response, the number of runs required to layout the experiment is large. This problem of large runs can be solved by considering fractional replication.

Example 2.2 Consider a 2^{4-1} factorial with four columns for four factors in 8 runs. Rotate the columns cyclically 3 times to obtain 32 points. Finally, add the first run at the bottom and last run at the top as border rows. The 32×5 matrix $\boldsymbol{X}$ of 4 predictor variables with first column of 1's, the coefficients of mean and two extra points as border points is obtained.

$$
\left|\begin{array}{rrrrr}
\hline
1 & 1 & 1 & -1 & 1 \\
\hline
1 & -1 & -1 & -1 & -1 \\
1 & -1 & -1 & 1 & 1 \\
1 & -1 & -1 & -1 & 1 \\
1 & -1 & 1 & 1 & -1 \\
1 & 1 & -1 & -1 & -1 \\
1 & 1 & -1 & 1 & 1 \\
1 & 1 & 1 & -1 & 1 \\
1 & 1 & 1 & 1 & -1 \\
\hline
\end{array}\right|
\left|\begin{array}{rrrrr}
\hline
1 & -1 & -1 & -1 & -1 \\
1 & 1 & -1 & -1 & 1 \\
1 & 1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & -1 \\
1 & 1 & 1 & -1 & 1 \\
1 & 1 & 1 & 1 & -1 \\
1 & -1 & 1 & 1 & 1 \\
\hline
\end{array}\right|
$$

$$
\left|\begin{array}{rrrrr}
\hline
1 & -1 & -1 & -1 & -1 \\
1 & 1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1 & 1 \\
1 & 1 & -1 & -1 & 1 \\
1 & -1 & -1 & 1 & -1 \\
1 & 1 & 1 & 1 & -1 \\
1 & -1 & 1 & 1 & 1 \\
1 & 1 & -1 & 1 & 1 \\
\hline
\end{array}\right|
\left|\begin{array}{rrrrr}
\hline
1 & -1 & -1 & -1 & -1 \\
1 & -1 & 1 & 1 & -1 \\
1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & -1 & -1 \\
1 & -1 & -1 & -1 & 1 \\
1 & -1 & 1 & 1 & 1 \\
1 & 1 & -1 & 1 & 1 \\
1 & 1 & 1 & -1 & 1 \\
\hline
1 & -1 & -1 & -1 & -1 \\
\hline
\end{array}\right|
$$

The variance of the parameter estimates and variance of the estimated response is obtained as $V(\hat{\beta}_0) = 0.0122\sigma^2, V(\hat{\beta}_i) = 0.0309\sigma^2$, and $V(\hat{y}_0) = 0.1360\sigma^2$. The values in the case of full factorial are $V(\hat{\beta}_0) = 0.0061\sigma^2, V(\hat{\beta}_i) = 0.0121\sigma^2$ and $V(\hat{y}_0) = 0.504\sigma^2$.

3. Second Order Response Surface Model with Differential Neighbour Effects

We consider the following form of $f(X_u)$:

$$f(X_u) = \beta_0 + \sum_{i=1}^{v} \beta_i X_{iu} + \sum_{i=1}^{v} \beta_{ii} X_{iu}^2 \tag{3.1}$$

$$\boldsymbol{X}_{(N+2)\times 5} = \left[\begin{array}{ccccc} 1 & X_{1N} & X_{2N} & X_{1N}^2 & X_{2N}^2 \\ \hline 1 & X_{11} & X_{21} & X_{11}^2 & X_{21}^2 \\ 1 & X_{12} & X_{22} & X_{12}^2 & X_{22}^2 \\ . & & & & \\ . & & & & \\ . & & & & \\ 1 & X_{1u} & X_{2u} & X_{1u}^2 & X_{2u}^2 \\ . & & & & \\ . & & & & \\ . & & & & \\ 1 & X_{1N} & X_{2N} & X_{1N}^2 & X_{2N}^2 \\ \hline 1 & X_{11} & X_{21} & X_{11}^2 & X_{21}^2 \end{array}\right] \tag{3.2}$$

Thus,

$\boldsymbol{Z'Z}$ is

$$\begin{bmatrix} pN & p\sum_{u=1}^{N} X_{1u} & p\sum_{u=1}^{N} X_{2u} & p\sum_{u=1}^{N} X_{1u}^2 & p\sum_{u=1}^{N} X_{2u}^2 \\ & q\sum_{u=1}^{N} X_{1u}^2 + A_1 & q\sum_{u=1}^{N} X_{1u}\ X_{2u} + C_1 & q\sum_{u=1}^{N} X_{1u}^3 + C_2 & q\sum_{u=1}^{N} X_{1u}\ X_{2u}^2 + C_3 \\ & & q\sum_{u=1}^{N} X_{2u}^2 + A_2 & q\sum_{u=1}^{N} X_{1u}^2 + C_4 & q\sum_{u=1}^{N} X_{2u}^3 + C_5 \\ & & & q\sum_{u=1}^{N} X_{2u}^4 + B_1 & q\sum_{u=1}^{N} X_{1u}^2 X2u^2 + D \\ & & & & q\sum_{u=1}^{N} X_{2u}^4 + B_2 \end{bmatrix}$$

where $p = (1+\alpha_1+\alpha_2)^2$ and $q = (1+\alpha_1^2+\alpha_2^2)$

where,

$$A_1 = 2\alpha_1\alpha_2 \left[\sum_{u=1}^{N} X_{1u}X_{1[(u+2)\ \mathrm{mod} N]}\right] + 2(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{1u}X_{1[(u+1)\ \mathrm{mod} N]}\right]$$

$$A_2 = 2\alpha_1\alpha_2 \left[\sum_{u=1}^{N} X_{2u}X_{2[(u+2)\ \mathrm{mod} N]}\right] + 2(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{2u}X_{2[(u+1)\ \mathrm{mod} N]}\right]$$

$$B_1 = 2\alpha_1\alpha_2 \left[\sum_{u=1}^{N} X_{1u}^2X_{1[(u+2)\ \mathrm{mod} N]}^2\right] + 2(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{1u}^2X_{1[(u+1)\ \mathrm{mod} N]}^2\right]$$

$$B_2 = 2\alpha_1\alpha_2 \left[\sum_{u=1}^{N} X_{2u}^2X_{2[(u+2)\ \mathrm{mod} N]}^2\right] + 2(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{2u}^2X_{2[(u+1)\ \mathrm{mod} N]}^2\right]$$

$$\begin{aligned}C_1 = \alpha_1\alpha_2 &\left[\sum_{u=1}^{N} X_{1u}X_{2[(u+2)\ \mathrm{mod} N]}\right] + \left[\sum_{u=1}^{N} X_{1[(u+2)\ \mathrm{mod} N]}X_{2u}\right]\\ &+(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{1u}X_{1[(u+1)\ \mathrm{mod} N]}^2 + \sum_{u=1}^{N} X_{1u}^2X_{1[(u+1)\ \mathrm{mod} N]}X_{2u}\right]\end{aligned}$$

$$\begin{aligned}C_2 = \alpha_1\alpha_2 &\left[\sum_{u=1}^{N} X_{1u}X_{1[(u+2)\ \mathrm{mod} N]}^2 + \sum_{u=1}^{N} X_{1u}^2X_{1[(u+2)\ \mathrm{mod} N]}\right]\\ &+(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{1u}X_{1[(u+1)\ \mathrm{mod} N]}^2 + \sum_{u=1}^{N} X_{1u}^2X_{1[(u+1)\ \mathrm{mod} N]}X_{2u}\right]\end{aligned}$$

$$\begin{aligned}C_3 = \alpha_1\alpha_2 &\left[\sum_{u=1}^{N} X_{1u}X_{2[(u+2)\ \mathrm{mod} N]}^2 + \sum_{u=1}^{N} X_{1[(u+2)\ \mathrm{mod} N]}X_{2u}^2\right]\\ &+(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{1u}X_{2[(u+1)\ \mathrm{mod} N]}^2 + \sum_{u=1}^{N} X_{1[(u+1)\ \mathrm{mod} N]}X_{2u}^2\right]\end{aligned}$$

$$\begin{aligned}C_4 = \alpha_1\alpha_2 &\left[\sum_{u=1}^{N} X_{1[(u+2)\ \mathrm{mod} N]}^2X_{2u} + \sum_{u=1}^{N} X_{1u}^2X_{2[(u+2)\ \mathrm{mod} N]}\right]\\ &+(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{1[(u+1)\quad \mathrm{mod}\ N]}^2X_{2u} + \sum_{u=1}^{N} X_{1u}^2X_{2[(u+1)\ \mathrm{mod} N]}\right]\end{aligned}$$

$$C_5 = \alpha_1\alpha_2 \left[\sum_{u=1}^{N} X_{2u}X^2_{[(u+2)\ \mathrm{mod} N]} + \sum_{u=1}^{N} X^2_{2u}X^2_{2[(u+2)\ \mathrm{mod} N]}\right]$$
$$+(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X_{2u}X^2_{2[(u+1)\ \mathrm{mod} N]} + \sum_{u=1}^{N} X^2_{2u}X_{2[(u+1)\ \mathrm{mod} N]}\right]$$

$$D = \alpha_1\alpha_2 \left[\sum_{u=1}^{N} X^2_{1u}X^2_{2[(u+2)\ \mathrm{mod} N]} + \sum_{u=1}^{N} X^2_{1[(u+2)\ \mathrm{mod} N]}X^2_{2u}\right]$$
$$+(\alpha_1+\alpha_2)\left[\sum_{u=1}^{N} X^2_{1u}X^2_{2[(u+1)\ \mathrm{mod} N]} + \sum_{u=1}^{N} X^2_{1[(u+1)\ \mathrm{mod} N]}X^2_{2u}\right]$$

For near-orthogonal estimation of parameters and constancy of variances of linear parameters and quadratic parameters, the following conditions are required:

i) $\sum_{u=1}^{N}\prod_{i=1}^{2} X^{\omega_i}_{iu} = 0$ for $\omega_i = 0, 1$ or 3 and $0 < \sum \omega_i < 4$

ii) $\sum_{u=1}^{N} X^2_{iu} = 0$ constant $N\eta = \delta, \qquad \forall\ i = 1, 2$

iii) $\sum_{u=1}^{N} X^2_{iu}X^2_{i'u} = \text{constant} = N\gamma = L$

iv) $\sum_{u=1}^{N} X^4_{iu} = \text{constant} = CL$

v) $A_i = A$ and $B_i = B \qquad \forall\ i = 1, 2.$ (3.3)

Therefore,

$$\boldsymbol{Z'Z} = \left[\begin{array}{cc|c} N(1+\alpha_1+\alpha_2)^2 & \mathbf{0'}_{1\times 2} & (1+\alpha_1+\alpha_2)^2\delta\mathbf{1'}_{1\times 2} \\ \mathbf{0'}_{2\times 1} & [(1+\alpha_1^2+\alpha_2^2)\delta + A]\boldsymbol{I}_2 & \mathbf{0}_{2\times 2} \\ \hline (1+\alpha_1+\alpha_2)^2\delta\mathbf{1}_{2\times 1} & \mathbf{0}_{2\times 2} & \boldsymbol{H}_{2\times 2} \end{array}\right]$$

Thus,

$$(\boldsymbol{Z'Z})^{-1} = \begin{bmatrix} \frac{1}{N(1+\alpha_1+\alpha_2)^2} + 2\frac{\delta}{N}\xi & \boldsymbol{0'}_{1\times 2} & -\xi\boldsymbol{1'}_{1\times 2} \\ \boldsymbol{0}_{2\times 1} & \frac{1}{[(1+\alpha_1^2+\alpha_2^2)\delta+A]}\boldsymbol{I}_2 & \boldsymbol{0}_{2\times 2} \\ -\xi\boldsymbol{1}_{2\times 1} & \boldsymbol{0}_{2\times 2} & \boldsymbol{\Psi}_{2\times 2} \end{bmatrix},$$

where,

$$\xi = \frac{\delta}{N}\left[\frac{[(1+\alpha_1^2+\alpha_2^2)L(C-1)+B-D]+[(1+\alpha_1^2+\alpha_2^2)L+D-\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2]}{\Delta}\right],$$

$$\boldsymbol{\Psi} = \left[\frac{(1+\alpha_1^2+\alpha_2^2)L(C+1)+B+D-2(1+\alpha_1^2+\alpha_2^2)\frac{\delta^2}{N}}{\Delta}\right]\boldsymbol{I}_2$$
$$+\left[-\frac{(1+\alpha_1^2+\alpha_2^2)L+D-\frac{delta^2}{N}(1+\alpha_1+\alpha_2)^2}{\Delta}\right]\boldsymbol{11'}$$

and

$$\Delta = [(1+\alpha_1^2+\alpha_2^2)L(C-1)+B-D]\{[(1+\alpha_1^2+\alpha_2^2)L(C-1)+B-D]$$
$$+2[(1+\alpha_1^2+\alpha_2^2)L+D-\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2]\}$$

The variances of the parameter estimates and covariances between the parameter estimates are obtained as

$$V(\hat{\beta}_0) = \frac{\sigma^2}{N(1+\alpha_1+\alpha_2)^2}\left[1+2\delta(1+\alpha_1+\alpha_2)^2\xi\right]$$
$$V(\hat{\beta}_i) = \frac{\sigma^2}{[(1+\alpha_1^2+\alpha_2^2)\delta+A]}, i=1,2 \tag{3.4}$$

$$V(\hat{\beta}_{ii}) = \sigma^2\frac{(1+\alpha_1^2+\alpha_2^2)L(C+1)+B+D-2(1+\alpha_1^2+\alpha_2^2)\frac{\delta^2}{N}}{\Delta}$$

$$\mathrm{Cov}(\hat{\beta}_0,\hat{\beta}_{ii}) = -\sigma^2\xi$$

$$\mathrm{Cov}(\hat{\beta}_{ii},\hat{\beta}_{i'i'}) = -\sigma^2\left[-\frac{(1+\alpha_1^2+\alpha_2^2)L+D-\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2}{\Delta}\right], i\neq i'$$

$$\mathrm{Cov}(\hat{\beta}_0,\hat{\beta}_{ii}) = 0$$

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

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

Thus,

$$V(\hat{y}_0) = V(\hat{\beta}_0) + V(\hat{\beta}_i)\sum_{i=1}^{v} x_{i0}^2 \; + V(\hat{\beta}_{ii})\sum_{i=1}^{v} x_{i0}^4$$

$$+2\ \mathrm{Cov}(\hat{\beta}_0, \hat{\beta}_{ii})\sum_{i=1}^{v} x_{i0}^2 \; + 2\ \mathrm{cov}(\hat{\beta}_{ii}, \hat{\beta}_{i'i'})\sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} x_{i0}^2\, x_{i'0}^2$$

Therefore,

$$V(\hat{y}_0)\sigma^{-2} = \frac{1}{N(1+\alpha_1+\alpha_2)^2}[1 + 2\delta(1+\alpha_1+\alpha_2)^2\xi]$$

$$+\{\frac{1}{[(1+\alpha_1^2+\alpha_2^2)\delta + A]} - 2\xi\} \sum_{i=1}^{v} x_{i0}^2$$

$$+\frac{(1+\alpha_1^2+\alpha_2^2)L(C+1) + B + D - 2(1+\alpha_1^2+\alpha_2^2)\frac{\delta^2}{N}}{\Delta} \sum_{i=1}^{v} x_{i0}^4$$

$$-2\frac{[(1+\alpha_1^2+\alpha_2^2)L + D - \frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2]}{\Delta} \sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} x_{i0}^2\, x_{i'0}^2$$

For v factors,

$$\boldsymbol{Z'Z} = \left[\begin{array}{cc|c} N(1+\alpha_1+\alpha_2)^2 & \boldsymbol{0'}_{1\times v} & (1+\alpha_1+\alpha_2)^2\delta\boldsymbol{1'}_{1\times v} \\ \boldsymbol{0'}_{v\times 1} & [(1+\alpha_1^2+\alpha_2^2)\delta + A]\boldsymbol{I}_v & \boldsymbol{0}_{v\times v} \\ \hline (1+\alpha_1+\alpha_2)^2\delta\boldsymbol{1}_{v\times 1} & \boldsymbol{0}_{v\times v} & \boldsymbol{H}_{v\times v} \end{array}\right]$$

with

$$(\boldsymbol{Z'Z})^{-1} = \begin{bmatrix} \frac{1}{N(1+\alpha_1+\alpha_2)^2} + 2\frac{\delta}{N}\xi & \boldsymbol{0'}_{1\times v} & -\xi\boldsymbol{1'}_{1\times v} \\ \boldsymbol{0}_{v\times 1} & \frac{1}{[(1+\alpha_1^2+\alpha_2^2)\delta+A]}\boldsymbol{I}_v & \boldsymbol{0}_{v\times v} \\ -\xi\boldsymbol{1}_{v\times 1} & \boldsymbol{0}_{v\times v} & \boldsymbol{\Psi} \end{bmatrix},$$

where,

$$\xi = \frac{\delta}{N}$$

$$\left[\frac{[(1+\alpha_1^2+\alpha_2^2)L(C-1)+B-D]+(v-1)\left[(1+\alpha_1^2+\alpha_2^2)L+D-\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2\right]}{\Delta}\right],$$

$$\boldsymbol{\Psi}=\left[\frac{(1+\alpha_1^2+\alpha_2^2)L(C+v-1)+B+(v-1)D-v\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2}{\Delta}\right]\boldsymbol{I}_v$$
$$+\left[-\frac{(1+\alpha_1^2+\alpha_2^2)L+D-\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2}{\Delta}\right]\mathbf{11'}$$

and

$$\Delta=\left[(1+\alpha_1^2+\alpha_2^2)L(C-1)+B-D\right]$$
$$\left\{\begin{array}{l}\left[(1+\alpha_1^2+\alpha_2^2)L(C-1)+B-D\right]+\\ v\left[(1+\alpha_1^2+\alpha_2^2)L+D-\frac{R^2}{N}(1+\alpha_1+\alpha_2)^2\right]\end{array}\right\}$$

Thus, expression for variances/covariances of the estimates are

$$V(\hat{\beta}_0)=\frac{\sigma^2}{N(1+\alpha_1+\alpha_2)^2}\left[1+v\delta(1+\alpha_1+\alpha_2)^2\xi\right]$$
$$V(\hat{\beta}_i)=\frac{\sigma^2}{[(1+\alpha_1^2+\alpha_2^2)\delta+A]}\text{ for } i=1,2\ldots,v$$
$$V(\hat{\beta}_{ii})=\sigma^2$$
$$\left[\frac{(1+\alpha_1^2+\alpha_2^2)L(C+v-1)+B+(v-1)D-v\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2}{\Delta}\right]$$
$$\mathrm{Cov}(\hat{\beta}_0,\hat{\beta}_{ii})=-\sigma^2\xi$$

$$\mathrm{Cov}(\hat{\beta}_{ii},\hat{\beta}_{i'i'})=\sigma^2\left[-\frac{(1+\alpha_1^2+\alpha_2^2)L+D-\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2}{\Delta}\right]$$
$$\mathrm{Cov}(\hat{\beta}_0,\hat{\beta}_i)=0 \tag{3.5}$$

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

$$V(\hat{y}_0)=V(\hat{\beta}_0)+V(\hat{\beta}_i)\sum_{i=1}^{v}x_{i0}^2\ +V(\hat{\beta}_{ii})\sum_{i=1}^{v}x_{i0}^4$$
$$+2\ \mathrm{Cov}(\hat{\beta}_0,\hat{\beta}_{ii})\sum_{i=1}^{v}x_{i0}^2\ +2\ \mathrm{cov}(\hat{\beta}_{ii},\hat{\beta}_{i'i'})\sum_{i=1}^{v-1}\sum_{i'=i+1}^{v}x_{i0}^2\,x_{i'0}^2$$

Using (3.5), we get

$$V(\hat{y}_0)\sigma^{-2} = \frac{1}{N(1+\alpha_1+\alpha_2)^2}[1+2\delta(1+\alpha_1+\alpha_2)^2\xi]$$

$$+\{\frac{1}{[(1+\alpha_1^2+\alpha_2^2)\delta+A]} - 2\xi\}\sum_{i=1}^{v} x_{i0}^2 +$$

$$\frac{(1+\alpha_1^2+\alpha_2^2)L(C+v-1)+B+(v-1)D-v\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2}{\Delta}\sum_{i=1}^{v} x_{i0}^4$$

$$-2\frac{[(1+\alpha_1^2+\alpha_2^2)L+D-\frac{\delta^2}{N}(1+\alpha_1+\alpha_2)^2]}{\Delta}\sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} x_{i0}^2\ x_{i'0}^2$$

A design under this situation is said to be rotatable if this variance is same for all points $\boldsymbol{x}$ which are equidistant from the design centre and the designs satisfying this property are called as Second Order Rotatable Designs with Differential Neighbour Effects (SORDDNE).

Remark : For $\alpha_1 = \alpha_2 = \alpha$, the above expression reduces to Sarika *et al.* (2009).

3.1 Method of Constructing SORDDNE

Considering the method given in section 2.1, construct a 3^v full factorial with levels $(-1, 0, 1)$ giving a rectangle R of 3^v rows and v columns with entries $-1, 0$ and 1. Circular rotation of the columns of $R, (v-1)$ times, yields $(v-1)$ sets each consisting of 3^v rows and v columns. By appending these sets below R one after another, we obtain a rectangular array of $v \times 3^v$ rows and v columns. Appending another $(v+1)$ columns (a column of unity and v columns of square terms), a SORDDNE in $v \times 3^v$ points is obtained by adding two extra points of border units such that each end of the array has a point of the other end.

Example 3.1 For $v = 2\,(X_1$ and $X_2)$, the design matrix, $\boldsymbol{X}$ in 18 points with two border points is as follows:

$$
\boldsymbol{X}_{20-5} = \left[\begin{array}{rrrrr}
1 & -1 & -1 & 1 & 1 \\ \hline
1 & 1 & 1 & 1 & 1 \\
1 & 0 & 1 & 0 & 1 \\
1 & -1 & 1 & 1 & 1 \\
1 & 1 & 0 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 \\
1 & -1 & 0 & 1 & 0 \\
1 & 1 & -1 & 1 & 1 \\
1 & 0 & -1 & 0 & 1 \\
1 & -1 & -1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 \\
1 & 1 & 0 & 1 & 0 \\
1 & 1 & -1 & 1 & 1 \\
1 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 \\
1 & 0 & -1 & 0 & 1 \\
1 & -1 & 1 & 1 & 1 \\
1 & -1 & 0 & 1 & 0 \\
1 & -1 & -1 & 1 & 1 \\ \hline
1 & 1 & 1 & 1 & 1
\end{array}\right]
$$

For $\alpha_1 = 0.6$ and $\alpha_2 = 0.4$

$$
\boldsymbol{Z}'\boldsymbol{Z} = \begin{bmatrix}
72 & 0 & 0 & 48 & 48 \\
0 & 16.8 & 0 & 0 & 0 \\
0 & 0 & 16.8 & 0 & 0 \\
48 & 0 & 0 & 37.6 & 32 \\
48 & 0 & 0 & 32 & 37.6
\end{bmatrix}
$$

Hence,

$$V(\hat{\beta}_0) = 0.172\sigma^2, V(\hat{\beta}_i) = 0.059\sigma^2, V(\hat{\beta}_{ii}) = 0.178\sigma^2,$$

$$\text{Cov } (\hat{\beta}_0, \hat{\beta}_{ii}) = -0.1090 \text{ and } V(\hat{y}_0) = 0.1726\sigma^2$$

Here, the variance of the estimated response is the same for all the points in the design and hence the design is rotatable.

4. Conclusions

The problem of neighbour effects is common in experiments conducted in the field. In response surface analysis, the presence of neighbour effect cannot be ignored as it may affect the precision of the parameter estimates of the model and hence of the estimated response. The methodology developed here may be useful to tackle the problem of neighbour effects and to get precise estimates of parameters. The technique has been illustrated through a simulated data set. Designs have been obtained for the experimental situations where neighbour effect is suspected. The design obtained here is considerably larger as compared to the designs used for fitting response surface without the neighbouring contamination, but this structure is needed to ensure proper estimation when neighbour effect is suspected.

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REFERENCES

Afsarinejad, K. (1990) Repeated measurements designs-A review. *Communication in Statistical Theory and Method* **19** 3985-4027.

Azais, J. M. and Druilhet, P. (1997). Optimality of neighbour balanced designs when neighbour effects are neglected. *J. Statistical Planning and Inference* **64** 353-367.

Azais, J. M., Bailey, R. A. and Monod, H. (1993). A catalogue of efficient neighbour design with border plots. *Biometrics* **49** 1252-1261.

Azais, J. M., Monod, H. and Bailey, R. A. (1998). The infuence of design on validity and efficiency of neighbour methods. *Biometrics* **54** 1374-1387.

Bailey, R. A. and Druilhet, P. (2004). Optimality of neighbour balanced designs for total effects. *The Ann. Statist.* **32** 1650-1661.

Bailey, R. A. (2003). Designs for one-sided neighbour effects. *J. Indian Soc. Agricultural Statist.* **56** 302-314.

Balaam, L. N. (1968). A two-period design with 2 experimental units. *Biometrics* 61-73.

Bartlett, M. S., (1978). Nearest neighbour models in the analysis of field experiments. *J. Royal Statistical Soc.* **40** 147-174.

Bose, M. and Dey, A. (2009). Optimal crossover designs. World Scientific Publishing Co. Pte. Ltd. Chennai, India.

Chan B. S. P. and Eccleston J. A. (2003). On the construction of nearest-neighbour balanced row-column designs, *Australian & New Zealand J. Statist.* **45** 97-106.

Dey, A. and Balachandran, G. (1976). A class of change-over designs balanced for first residual effects. *J. Indian Soc. Agricultural Statist.* **28** 57-64.

Draper, N. R., Guttman, I., (1980). Incorporating overlap effects from neighbouring units into response surface models. *Appl. Statist.* **29** 128-134.

Druilhet P. (1999). Optimality of neighbour balanced designs, *J. Statist. Plann. Inference* **81** 141-152.

Federer W. T. and Basford K. E. (1991). Competing effects designs and models for two-dimensional field arrangements, *Biometrics* **47** 1461-1472.

Freeman G. H. (1979). Some two dimensional designs balanced for nearest neighbours, *J. Royal Statistical Soc.* **41** 88-95.

Jaggi S., Varghese, C. and Gupta V. K. (2007). Optimal block designs for neighbouring competition effects. *J. Applied Statist.* **34** 577-584.

Jaggi, S., Gupta, V. K. and Ashraf, J. (2006). On block designs partially balanced for neighbouring competition effects. *J. Indian Statist. Assoc.* **44** 27-41.

Jaggi, S., Varghese, C., Varghese, E. and Sharma, A. (2015). Web generation of experimental designs balanced for indirect effects of treatments (WEB-DBIE). *Computers and Electronics in Agriculture* **111** 62-68.

Jaggi, Seema, Sarika and Sharma, V. K. (2010). Response surface analysis incorporating neighbour effects from adjacent units. *Indian J. Agricultural Sciences* **80** 719-723.

Khuri, A. I. and Cornell, J. A., (1996) Response Surfaces-Designs and Analysis. Marcel Dekker, New York.

Monod, H. and Bailey R. A. (1993). Two factor designs balanced for the neighbour effects on one factor. *Biometrika* **80** 643-659.

Montgomery, D. C. and Peck, E. A. (2006). Introduction to Linear Regression Analysis. John Wiley & Sons, New York.

Myers, R. H., Montgomery, D. C. and Andersson, C. M., (2009). Response Surface Methodology-Process and Product Optimization using Designed Experiments. New York, John Wiley Publication.

Pateria, D. K., Jaggi, S., Varghese, C. and Das, M. N. (2007). Incomplete non-circular block designs for competition effects. *Statistical and Applications* **5** 5-14.

Patterson, H. D. and Lucas, H. L. (1962). Change-over designs. *N. C. Agri. Exp. Station. Tech. Bull.* **147**.

Sarika, Jaggi, Seema, Sharma, V.K., (2008). First order rotatable designs incorporating neighbour effects. *ARS Combinatoria* **112** 145-160.

Sarika, Jaggi, Seema and Sharma, V. K., (2009). Second order response surface model with neighbour effects. *Communications in Statistics : Theory and Methods* **38** 1393-1403.

Sharma, A., Varghese, C. and Jaggi, S. (2013). A web solution for Partially Balanced Incomplete Block experimental designs. *Computer and Electronics in Agriculture* **99** 132-134.

Sharma, V. K. (1975). An easy method of constructing Latin square designs balanced for the immediate residual and other order effects. *Canadian J. Statist.* **2** 119-124.

Sharma, V. K. (1981). A class of experimental designs balanced for first residuals. *Austral. J. Statist.* **23** 365-370.

Sharma, V. K. (1982). Extra-period balanced change-over designs. *Sankhya* **44** 167-175.

Sharma, V. K., Jaggi, S. and Varghese, C. (2003). Minimal balanced repeated measurements designs. *J. Applied Statist.* **30** 867-872.

Sharma, V. K., Varghese, C. and Jaggi, S. (2002). On optimality of change over designs balanced for first and second order residual effects. *Metron* **60** 155-164.

Tomar, J. S., Jaggi, S. and Varghese, C. (2005). On totally balanced block designs for competition effects. *J. Applied Statist.* **32** 87-97.

Varghese, C. and Sharma, V. K. (2000). On totally balanced change-over designs. *J. Indian Soc. Ag. Statist.* **53** 141-150.

Varghese, E., Jaggi, S. and Varghese, C. (2011). Row-column designs balanced for non-directional neighbour effects. *Model Assisted Statistics and Applications* **6** 307-316.

Varghese, E., Jaggi, S. and Varghese, C. (2014). Neighbor-Balanced Row-column Designs, *Communications in Statistics - Theory and Methods* **43** 1261-1276.

Williams, E. J. (1949). Experimental designs balanced for the estimation of residual effects of treatments. *Austral. J. Science Res.* **2** 149-168.