
Rotatable response surface designs for $s_1^{n_1} \times s_2^{n_2}$ incorporating neighbour effects

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Abstract:

- This paper describes the response surface methodology for mixed-level factors of the form $s_1^{n_1} \times s_2^{n_2}$ when experimental units experiences overlap effects from the adjacent neighbouring units. Conditions have been derived for the near orthogonal estimation of the parameters of the model and ensuring the constancy in the prediction variance. A method of construction of designs satisfying derived conditions has been developed. Some particular cases of $s_1^{n_1} \times s_2^{n_2}$ has also described. An R package named *rsdNE* has also been developed for the generation of these designs.

Keywords:

- *Mixed-level response surface design, neighbour effect, rotatable design.*

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1. INTRODUCTION

The response surface methodology (RSM) is a widely used statistical method for modelling and analyzing a process in which the response of interest is affected by various input variables, and the objective of this method is to optimize the response [3]. The main idea of RSM is to use a sequence of designed experiments to obtain an optimal response. If x_1, x_2, \dots, x_v are v independent variables, y is the response variable, and N is the total number of observations, then the response function can be approximated in some region of the polynomial model given by

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

where $u = 1, 2, \dots, N$, y_u is the response from u^{th} treatment combination and x_{iu} is the level of the i^{th} ($i = 1, 2, \dots, v$) factor in the u^{th} combination. The function $f(\cdot)$ describes the form in which the response and the input variables are related. e_u is the random error associated with the u th observation that is independently and normally distributed as $e_u \sim N(0, \sigma^2)$. For details on RSM, one can refer to [4], [8], [10], [11].

In RSM, it is mainly assumed that the observations are independent and that neighbouring units have no effect. But in agricultural field trials, the neighbouring effect or overlap effect is very prominent ([1], [2], [5], [6], [12]). For example, if a chemical treatment is sprayed on one plot, wind drift may allow the spray to spread to adjacent/neighbouring plots, or preceding soil preparation may allow sterilized soil from one plot to mingle with non-sterile soil from the next plot. As a result, it is vital to assume that the response received from a given plot is influenced not only by the treatment combinations used on that plot but also by the treatment combinations used on the plots next to it. So, it gives a great scope to take into account the neighbouring effects in RSM. Because of these neighbouring effects, the variation of treatment differences arises. If the neighbour effect is present and is included in the model, there is a considerable reduction in the residual sum of squares, and the response is predicted with more precision [7]. Over the years, work on different aspects of RSM with neighbour effects from immediate adjacent neighbours has been done for factors with same levels ([13], [14], [15], [16], [17], [18]). The response surface model with neighbour effects up to distance 2 has also available in the literature [9]. Some attempts were also made to develop asymmetrical response surface designs of the form $2^n \times 3$ and $2^n \times 3^n$ in the presence of neighbour effects [19].

Here, a general methodology for constructing response surface designs of

the form $s_1^{n_1} \times s_2^{n_2}$ has been developed, incorporating neighbour effects and an R package named *rsdNE* has also been developed for the generation of these designs.

2. Response Surface Model with Neighbour Effects

Consider a response surface with n_1 factors at s_1 levels each and n_2 factors at s_2 levels each resulting in $s_1^{n_1} \times s_2^{n_2}$ combinations. The form $f(x_u)$ of considered here is as follows:

$$f(x_u) = \beta_0 + \sum_{i=1}^{n_1} \beta_i x_i + \sum_{i=n_1+1}^{n_1+n_2} \beta_i x_i + \sum_{i=1}^{n_1} \beta_{ii} x_i^2 + \sum_{i=n_1+1}^{n_1+n_2} \beta_{ii} x_i^2 + \dots +$$

$$(2.1) \quad \sum_{i=1}^{n_1} \beta_{ii\dots i} x_i^{s_1-1} + \sum_{i=n_1+1}^{n_1+n_2} \beta_{ii\dots i} x_i^{s_2-1}$$

where β_0, β_i 's [associated with linear terms of $n_1 + n_2$ factors], β_{ii} [associated with quadratic term of $n_1 + n_2$ factors] and $\beta_{ii\dots i}$ [associated with $(s_i - 1)^{th}$ order term of n_i^{th} factor] are parameters to be estimated. Thus, the total number of parameters to be estimated in above model is $p = n_1(s_1 - 1) + n_2(s_2 - 1) + 1$. The response model incorporating the effects from immediate left and right neighbouring units is defined as follows:

$$(2.2) \quad y_{u'} = \sum_{u=1}^N g_{uu'} f(x_u) + e_{u'}, u' = 1, 2, \dots, N$$

where,

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

Here, α represents the neighbour effect from left and right neighbouring units and ranges from 0 to 1 ([6], [13]). $f(x_u)$ is as given in 2.1.

It is to be mentioned that the design layout of the experiment for estimating this model will consist of two extra units as border units at each end. Observations are not taken from border units and thus are not modelled.

Model 2.2 can be rewritten as

$$(2.3) \quad \mathbf{Y} = \mathbf{G}\mathbf{X}\mathbf{Y} + \mathbf{e},$$

where $\mathbf{G} = g_{uu'}$ is the $N \times (N + 2)$ symmetric neighbour matrix, \mathbf{X} is a $(N + 2) \times p$

matrix of N points (runs) with two extra border units (treatment combinations applied on these units are the treatment combinations from the N points), p is the number of parameters, $\boldsymbol{\beta}$ is a $p \times 1$ vector of parameters to be estimated and \mathbf{e} is $N \times 1$ vector of errors which follows $N(0, \sigma^2 \mathbf{I})$

The ordinary least squares estimate of $\boldsymbol{\beta}$, in the presence of neighbour effects with known \mathbf{G} is

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

where, $\mathbf{Z}=\mathbf{B}\mathbf{X}$ and $D(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{Z}'\mathbf{Z})^{-1}$

2.1. Response Surface Methodology for $3^2 \times 4^2$ with Neighbour Effects

Consider $n_1 = n_2 = 2, s_1 = 3, s_2 = 4$ i.e. 2 factors at levels two and 2 factors at levels four. The form of $f(x_u)$ is as follows:

$$(2.4) \quad f(x_u) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{44} x_4^2 + \beta_{333} x_3^3 + \beta_{444} x_4^3$$

The matrix \mathbf{X} in 2.3 is here as follows of order $(N + 2) \times 11$ with two border units:

$$\mathbf{X}_{(N+2) \times 11} = \begin{bmatrix} 1 & x_{1N} & x_{2N} & \dots & x_{4N}^2 & x_{3N}^3 & x_{4N}^3 \\ \mathbf{1} & \mathbf{X}_1 & \mathbf{X}_2 & \dots & \mathbf{X}_4^2 & \mathbf{X}_3^3 & \mathbf{X}_4^3 \\ 1 & x_{11} & x_{21} & \dots & x_{41}^2 & x_{31}^3 & x_{41}^3 \end{bmatrix}$$

where, $\mathbf{X}_i^b = [x_{i1}^b \ x_{i2}^b \ \dots \ x_{iN}^b]'$; $\mathbf{X}_i^1 = \mathbf{X}_i$, $i = 1, 2, 3, 4$ and $b = 1, 2, 3$; and $\mathbf{1}_N = [1 \ 1 \ \dots \ 1]'$ The structure of \mathbf{G} matrix is

$$\mathbf{G}_{N \times (N+2)} = \begin{bmatrix} \alpha & 1 & \alpha & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & \alpha & 1 & \alpha & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \alpha & 1 & \alpha & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \alpha & 1 & \alpha & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \alpha & 1 & \alpha & 0 \\ 0 & 0 & 0 & 0 & 0 & \dots & \alpha & 1 & \alpha \end{bmatrix}$$

Further, $\mathbf{Z} = \mathbf{G}\mathbf{X} =$

$$\begin{bmatrix} \theta' & x_{11} + \alpha(x_{1N} + x_{12}) & \dots & x_{31}^2 + \alpha(x_{3N}^2 + x_{32}^2) & \dots & x_{41}^3 + \alpha(x_{4N}^3 + x_{42}^3) \\ \theta' & x_{12} + \alpha(x_{11} + x_{13}) & \dots & x_{32}^2 + \alpha(x_{31}^2 + x_{33}^2) & \dots & x_{42}^3 + \alpha(x_{41}^3 + x_{43}^3) \\ \theta' & x_{13} + \alpha(x_{12} + x_{14}) & \dots & x_{33}^2 + \alpha(x_{32}^2 + x_{34}^2) & \dots & x_{43}^3 + \alpha(x_{42}^3 + x_{44}^3) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \theta' & x_{1(N-1)} + \alpha(x_{1N} + x_{1(N-2)}) & \dots & x_{3(N-1)}^2 + \alpha(x_{3N}^2 + x_{3(N-2)}^2) & \dots & x_{4(N-1)}^3 + \alpha(x_{4N}^3 + x_{4(N-2)}^3) \\ \theta' & x_{1N} + \alpha(x_{11} + x_{1(N-1)}) & \dots & x_{3N}^2 + \alpha(x_{31}^2 + x_{3(N-1)}^2) & \dots & x_{4N}^3 + \alpha(x_{41}^3 + x_{4(N-1)}^3) \end{bmatrix}$$

where, $\theta' = 1 + 2\alpha$.

$$\mathbf{Z}'\mathbf{Z} = \begin{bmatrix} N\theta_1 & \theta_1 \sum_{u=1}^N x_{1u} & \cdots & \theta_1 \sum_{u=1}^N x_{3u}^3 & \theta_1 \sum_{u=1}^N x_{4u}^3 \\ \theta_2 \sum_{u=1}^N x_{1u}^2 + A_1 & \cdots & \theta_2 \sum_{u=1}^N x_{1u}x_{3u}^3 + D_1 & \theta_2 \sum_{u=1}^N x_{1u}x_{4u}^3 + D_2 & \\ & \ddots & \vdots & \vdots & \\ & & \theta_2 \sum_{u=1}^N x_{3u}^6 + G_1 & \theta_2 \sum_{u=1}^N x_{3u}^3x_{4u}^3 + G_2 & \\ & & & \theta_2 \sum_{u=1}^N x_{4u}^6 + G_3 & \end{bmatrix}$$

where, $\theta_1 = (1 + 2\alpha)^2$ and $\theta_2 = (1 + 2\alpha^2)$

$$A_i = 2\alpha^2 \sum_{u=1}^N x_{iu}x_{i(u+2)\text{mod}(N)} + 4\alpha \sum_{u=1}^N x_{iu}x_{i(u+1)\text{mod}(N)}$$

$$B_i = 2\alpha^2 \sum_{u=1}^N x_{iu}^2x_{i(u+2)\text{mod}(N)}^2 + 4\alpha \sum_{u=1}^N x_{iu}^2x_{i(u+1)\text{mod}(N)}^2$$

$$G_g = 2\alpha^2 \sum_{u=1}^N x_{iu}^3x_{i(u+2)\text{mod}(N)}^3 + 4\alpha \sum_{u=1}^N x_{iu}^3x_{i(u+1)\text{mod}(N)}^3$$

$$O_k = \alpha^2 \left(\sum_{u=1}^N x_{iu}x_{j(u+2)\text{mod}(N)} + \sum_{u=1}^N x_{i(u+2)\text{mod}(N)}x_{ju} \right) + 2\alpha \left(\sum_{u=1}^N x_{iu}x_{j(u+1)\text{mod}(N)} + \sum_{u=1}^N x_{iu}x_{j(u-1)\text{mod}(N)} \right)$$

$$C_k = \alpha^2 \left(\sum_{u=1}^N x_{iu}x_{j(u+2)\text{mod}(N)}^2 + \sum_{u=1}^N x_{i(u+2)\text{mod}(N)}x_{ju}^2 \right) + 2\alpha \left(\sum_{u=1}^N x_{iu}x_{j(u+1)\text{mod}(N)}^2 + \sum_{u=1}^N x_{iu}x_{j(u-1)\text{mod}(N)}^2 \right)$$

$$F_k = 2\alpha^2 \sum_{u=1}^N x_{iu}^2x_{j(u+2)\text{mod}(N)}^2 + 4\alpha \sum_{u=1}^N x_{iu}^2x_{j(u+1)\text{mod}(N)}^2$$

$$E_m = \alpha^2 \left(\sum_{u=1}^N x_{iu}^2x_{j(u+2)\text{mod}(N)}^3 + \sum_{u=1}^N x_{i(u+2)\text{mod}(N)}^2x_{ju}^3 \right) + 2\alpha \left(\sum_{u=1}^N x_{iu}^2x_{j(u+1)\text{mod}(N)}^3 + \sum_{u=1}^N x_{iu}^2x_{j(u-1)\text{mod}(N)}^3 \right)$$

$$D_m = \alpha^2 \left(\sum_{u=1}^N x_{iu}x_{j(u+2)\text{mod}(N)}^3 + \sum_{u=1}^N x_{i(u+2)\text{mod}(N)}x_{ju}^3 \right) + 2\alpha \left(\sum_{u=1}^N x_{iu}x_{j(u+1)\text{mod}(N)}^3 + \sum_{u=1}^N x_{iu}x_{j(u-1)\text{mod}(N)}^3 \right)$$

where,

$$\begin{aligned}
g_{11} &= f_{11}\theta_1\delta_1 + f_{12}\theta_1\delta_2 + f_{13}\theta_1\delta_3 + f_{14}\theta_1\delta_4 \\
f_{11} &= E^{11}\theta_1\delta_1 + E^{12}\theta_1\delta_2 + E^{13}\theta_1\delta_3 - C_{11}K_{11}\theta_1\delta_4 \\
f_{12} &= E^{12}\theta_1\delta_1 + E^{22}\theta_1\delta_2 + E^{32}\theta_1\delta_3 - C_{11}K_{12}\theta_1\delta_4 \\
f_{13} &= E^{13}\theta_1\delta_1 + E^{23}\theta_1\delta_2 + E^{33}\theta_1\delta_3 - C_{11}K_{13}\theta_1\delta_4 \\
f_{14} &= -C_{11}K_{11}\theta_1\delta_1 - C_{11}K_{12}\theta_1\delta_2 - C_{11}K_{13}\theta_1\delta_3 - C_{11}\theta_1\delta_4 \\
E_{11} &= \theta_2\delta_1 + B_1 - \frac{\delta_1^2\theta_1}{N} \\
E_{12} &= \theta_2\lambda_1 + F_1 - \frac{\delta_1\delta_2\theta_1}{N} = E_{12} \\
E_{13} &= \theta_2\lambda_1 + F_2 - \frac{\delta_1\delta_3\theta_1}{N} = E_{31} \\
E_{22} &= \theta_2\gamma_2 + B_2 - \frac{\delta_2^2\theta_1}{N} \\
E_{23} &= \theta_2\lambda_1 + F_4 - \frac{\delta_2\delta_3\theta_1}{N} = E_{32} \\
E_{33} &= \theta_2\delta_3 + B_3 - \frac{\delta_3^2\theta_1}{N} \\
E_{55} &= \theta_2\beta_3 + G_1 \\
E_{56} &= \theta_2\lambda_2 + G_2 \\
E_{66} &= \theta_2\beta_2 + G_3
\end{aligned}$$

$$E_1 = \begin{bmatrix} E_{44} & -(E_{14}K_{11} + E_{24}K_{12} + E_{34}K_{13}) & 0 & 0 \\ & E_{55} & E_{56} & \\ & & E_{66} & \end{bmatrix} K_1 = \begin{bmatrix} E_{11} & E_{12} & E_{13} \\ & E_{22} & E_{23} \\ & & E_{33} \end{bmatrix}$$

$$C_{11} = \frac{(E_{55}E_{66} - E_{65}E_{56})}{|E_1|}$$

$$C_{22} = E_{66}\nabla$$

$$C_{33} = E_{55}\nabla$$

$$C_{23} = E_{65}\nabla$$

$$K_{11} = \frac{(E_{41}(E_{21}E_{33} - E_{23}^2) + E_{42}(E_{13}E_{33} - E_{12}E_{23}) + E_{43}M(E_{13}))}{|K_1|}$$

$$K_{12} = \frac{(E_{41}M(E_{13}) + E_{42}M(E_{22}) + E_{43}M(E_{32}))}{|K_1|}$$

$$K_{13} = \frac{(E_{41}M(E_{13}) + E_{42}M(E_{23}) + E_{43}M(E_{33}))}{|K_1|}$$

where, $\nabla = \frac{[E_{44} - (E_{14}K_{11} + E_{24}K_{12} + E_{34}K_{13})]}{|E_1|}$ and $M(E_{ij}) = \text{minor of } E_{ij}$

The expressions of the variance and covariance terms of the estimates are given

below

$$\begin{aligned}
Var(\hat{\beta}_0) &= \frac{1}{N\theta_1} + g_{11} & Var(\hat{\beta}_{11}) &= E^{11} \\
Var(\hat{\beta}_1) &= \frac{1}{\theta_2\delta_1 + A_1} & Var(\hat{\beta}_{22}) &= E^{22} \\
Var(\hat{\beta}_2) &= \frac{1}{\theta_2\delta_2 + A_2} & Var(\hat{\beta}_{33}) &= E^{33} \\
Var(\hat{\beta}_3) &= \frac{1}{\theta_2\delta_3 + A_3} & Var(\hat{\beta}_{44}) &= -C_{11} \\
Var(\hat{\beta}_4) &= \frac{1}{\theta_2\delta_4 + A_4} & Var(\hat{\beta}_{333}) &= C_{22} \\
& & Var(\hat{\beta}_{444}) &= C_{33}
\end{aligned}$$

$$\begin{aligned}
Cov(\hat{\beta}_0, \hat{\beta}_{11}) &= -f_{11} & Cov(\hat{\beta}_{22}, \hat{\beta}_{333}) &= -C_{11}K_{11} \\
Cov(\hat{\beta}_0, \hat{\beta}_{22}) &= -f_{12} & Cov(\hat{\beta}_{33}, \hat{\beta}_{44}) &= E^{23} \\
Cov(\hat{\beta}_0, \hat{\beta}_{33}) &= -f_{13} & Cov(\hat{\beta}_{33}, \hat{\beta}_{333}) &= -C_{11}K_{12} \\
Cov(\hat{\beta}_0, \hat{\beta}_{44}) &= -f_{14} & Cov(\hat{\beta}_{44}, \hat{\beta}_{333}) &= -C_{11}K_{13} \\
Cov(\hat{\beta}_{22}, \hat{\beta}_{33}) &= E^{12} & Cov(\hat{\beta}_{44}, \hat{\beta}_{444}) &= -C_{32} \\
& & Cov(\hat{\beta}_{22}, \hat{\beta}_{44}) &= E^{13}
\end{aligned}$$

$$\begin{aligned}
E^{11} &= (E_{21}E_{33} - E_{23}^2) + C_{11}K_{11}^2 & E^{12} &= M(E_{21}) + C_{11}K_{11}K_{12} = E^{21} \\
E^{13} &= M(E_{13}) + C_{11}K_{11}K_{13} = E^{31} & E^{22} &= M(E_{22}) + C_{11}K_{12}^2 \\
E^{33} &= M(E_{33}) + C_{11}K_{13}^2 & E^{23} &= M(E_{23}) + C_{11}K_{12}K_{13} = E^{32}
\end{aligned}$$

The estimated response at any point \mathbf{x}_0 is given below

$$\hat{y}_0 = \hat{\beta}_0 + \sum_{i=1}^4 \hat{\beta}_i x_{i0} + \sum_{i=1}^4 \hat{\beta}_{ii} x_{i0}^2 + \sum_{i=3}^4 \hat{\beta}_{iii} x_{i0}^3$$

with the variance of estimated response as

$$V(\hat{y}_0) = \sigma^2 \left[\begin{array}{l} V_0 + x_{10}^2 V_1 + x_{20}^2 V_2 + x_{30}^2 V_3 + x_{40}^2 V_4 + V_{11}x_{10}^4 + V_{22}x_{20}^4 + V_{33}x_{30}^4 + V_{44}x_{40}^4 + V_{333}x_{30}^6 \\ + V_{444}x_{40}^6 + 2C_{0,11}x_{10}^2 + 2C_{0,22}x_{20}^2 + 2C_{0,33}x_{30}^2 + 2C_{0,44}x_{40}^2 + 2C_{22,33}x_{20}^2x_{30}^2 + 2C_{22,44}x_{20}^2x_{40}^2 \\ + 2C_{22,333}x_{20}^2x_{30}^6 + 2C_{33,44}x_{30}^4x_{40}^4 + 2C_{33,333}x_{30}^{10} + 2C_{44,333}x_{40}^4x_{30}^6 + 2C_{44,444}x_{40}^{10} \end{array} \right]$$

where, $V_i = V(\hat{\beta}_i)$, $V_{ij} = V(\hat{\beta}_{ij})$ and so on. Similarly, $C_{i,j} = Cov(\hat{\beta}_i, \hat{\beta}_j)$, $C_{i,jk} =$

$Cov(\hat{\beta}_i, \hat{\beta}_{jk})$ and so on.

It can be seen that the variance of the estimated response at any point \mathbf{x}_0 depends on the distance of that point from the design centre. The design obtained for fitting this model with mixed levels of factors will be called here as Mixed Level Response Surface Design with Neighbour Effects. From this one can check, at any point \mathbf{x}_0 , the variance of the estimated response from the centre. If this is equal, then the design obtained is called as Mixed Level Rotatable Design with Neighbour Effects (MLRDNE) and if different, then partially rotatable. Similarly, this can be extended for $s_1^{n_1} \times s_2^{n_2}$.

The above discussions lead to the following theorem:

Theorem 1: A $s_1^{n_1} \times s_2^{n_2}$ mixed-level factorial arranged in reverse lexicographic order along with the circular borders at each end will lead to MLRDNE under the model defined in 2.2 with $f(x_u)$ as defined in 2.1, provided either s_1 or s_2 should be an odd number. The proof of theorem 1 has been given in the subsequent section with the help of examples.

3. Method of Constructing MLRDNE for $s_1^{n_1} \times s_2^{n_2}$

Consider n_1 factors having s_1 levels and n_2 factors having s_2 levels. The $n_1 + n_2$ columns of \mathbf{X} corresponding to $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{n_1}, \mathbf{X}_{n_1+1}, \dots, \mathbf{X}_{n_1+n_2}$ of MLRDNE in $N = \max(n_1, n_2) \times s_1^{n_1} \times s_2^{n_2}$ points are developed as follows:

$$\mathbf{X} = [\mathbf{O}_{N \times n_1} \quad \mathbf{Q}_{N \times n_2}]$$

$$\mathbf{O} = \begin{bmatrix} \mathbf{o}_1 & \mathbf{o}_2 & \cdots & \mathbf{o}_{n_1} \\ \mathbf{o}_{n_1} & \mathbf{o}_1 & \cdots & \mathbf{o}_{n_1-1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{o}_2 & \mathbf{o}_3 & \cdots & \mathbf{o}_1 \end{bmatrix} \quad \mathbf{Q} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_{n_2} \\ \mathbf{q}_{n_2} & \mathbf{q}_1 & \cdots & \mathbf{q}_{n_2-1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{q}_2 & \mathbf{q}_3 & \cdots & \mathbf{q}_1 \end{bmatrix}$$

\mathbf{o}_i and \mathbf{q}_j are the vectors of order $N' \times 1$ (where, $N' = s_1^{n_1} \times s_2^{n_2}$)

$\mathbf{o}_i = \mathbf{1}_{s_1^p \times s_2^{n_2}} \otimes (\text{column vector of } s_1 \text{ levels}) \otimes \mathbf{1}_{s_1^{n_1-i}}$; $p = i - 1, i = 1, 2, \dots, n_1 (> 1)$

$\mathbf{q}_j = \mathbf{1}_{s_1^{n_1} \times s_2^q} \otimes (\text{column vector of } s_2 \text{ levels}) \otimes \mathbf{1}_{s_2^{n_2-j}}$; $q = j - 1, j = 1, 2, \dots, n_2 (> 1)$

If $n_1 = 1$, then $\mathbf{O} = [\mathbf{o}_1 \quad \mathbf{o}_1]'$ and if $n_2 = 1$, then $\mathbf{Q} = [\mathbf{q}_1 \quad \mathbf{q}_1]'$

The other columns of \mathbf{X} are generated as per the model and values of s_1 and s_2 .

D-efficiency of the design can be calculated using the formula,

$$\frac{|\mathbf{Z}'\mathbf{Z}|^{\frac{1}{p}}}{N}$$

where, p is number of parameters considered in a model and N is total number of runs[19].

Example 3.1: Let $n_1 = n_2 = 2, s_1 = 2$ (levels: 1, -1) and $s_2 = 5$ (levels: 2, 1, 0, -1, -2) *i.e.* $2^2 \times 5^2$. The first four columns of \mathbf{X} corresponding to $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3$ and \mathbf{X}_4 and $2(2^2 \times 5^2) = 200$ points are as follows:

$$\mathbf{X} = [\mathbf{O}_{200 \times 2} \quad \mathbf{Q}_{200 \times 2}]$$

The other columns of \mathbf{X} are generated as per model with 11 columns ($\mathbf{1}, \mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_4, \mathbf{X}_3^2, \mathbf{X}_4^2, \mathbf{X}_3^3, \mathbf{X}_4^3, \mathbf{X}_3^4, \mathbf{X}_4^4$). For $\alpha = 0.5$,

$$\mathbf{Z}'\mathbf{Z} = \begin{bmatrix} 800 & \mathbf{0}'_2 & \mathbf{0}'_2 & 1600\mathbf{1}'_2 & \mathbf{0}'_2 & 5440\mathbf{1}'_2 \\ & 100\mathbf{I}_2 & \mathbf{O}_2 & \mathbf{O}_2 & \mathbf{O}_2 & \mathbf{O}_2 \\ & & 930\mathbf{I}_2 & \mathbf{O}_2 & 2910\mathbf{I}_2 & \mathbf{O}_2 \\ & & & \mathbf{A} & \mathbf{O}_2 & \mathbf{B} \\ & & & & 10074\mathbf{I}_2 & \mathbf{O}_2 \\ & & & & & \mathbf{C} \end{bmatrix}$$

where, $\mathbf{A} = 1470\mathbf{I}_2 + 3200\mathbf{J}_2$, $\mathbf{B} = 6438\mathbf{I}_2 + 10880\mathbf{J}_2$, $\mathbf{C} = 28686\mathbf{I}_2 + 36992\mathbf{J}_2$; \mathbf{I}_2 is identity matrix order 2×2 , \mathbf{J}_2 is matrix of 1's of order 2×2 , $\mathbf{1}$ is column vector of 1's of order 2×1 , $\mathbf{0}$ is a column vector of 0's of order 2×1 and \mathbf{O} is matrix of 0's of order 2×2 .

$$(\mathbf{Z}'\mathbf{Z})^{-1} = \begin{bmatrix} 0.02 & \mathbf{0}'_2 & \mathbf{0}'_2 & -0.021\mathbf{1}'_2 & \mathbf{0}'_2 & 0.0041\mathbf{1}'_2 \\ & 0.01\mathbf{I}_2 & \mathbf{O}_2 & \mathbf{O}_2 & \mathbf{O}_2 & \mathbf{O}_2 \\ & & 0.011\mathbf{I}_2 & \mathbf{O}_2 & -0.003\mathbf{I}_2 & \mathbf{O}_2 \\ & & & 0.004\mathbf{I}_2 & \mathbf{O}_2 & -0.009\mathbf{I}_2 \\ & & & & 0.001\mathbf{I}_2 & \mathbf{O}_2 \\ & & & & & 0.002\mathbf{I}_2 \end{bmatrix}$$

The variance of estimated response, $V(\hat{y}_0) = 0.042\sigma^2$ for all points in \mathbf{X} and so design is rotatable.

The method discussed in Section 3 leads to the following proposition:

Proposition 1: As the $V(\hat{y}_0)$ is the same for all points in \mathbf{X} which are equidistant from the design centre for $s_1^{n_1} \times s_2^{n_2}$ mixed-level factorial constructed as per the method given in 3, the design satisfies theorem 1 and hence rotatable.

For $\alpha = 0.5$, the eigen values of $(\mathbf{Z}'\mathbf{Z})^{-1}$ are 0.06, 0.042, 0.012, 0.012, 0.01, 0.01, 0.003, 9.1×10^{-5} , 9.1×10^{-5} , 3.3×10^{-5} , 9×10^{-6} and D-efficiency of this design is 2.979. At $\alpha = 0.1$, D-efficiency of this design is 1.958.

Remark 3.1: If s_1 and s_2 both are even, the design is partially rotatable.

3.1. Particular Cases of $s_1^{n_1} \times s_2^{n_2}$

3.1.1. For $n_2 = 1$, i.e. $s_1^{n_1} \times s_2$

Consider n_1 factors having s_1 levels and one factor having s_2 levels. The $n_1 + 1$ columns of \mathbf{X} corresponding to $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{n_1}, \mathbf{X}_{n_1+1}$ of MLRDNE in $N = n_1(s_1^{n_1} \times s_2)$ points are developed as follows:

$$\mathbf{X} = [\mathbf{O}_{N \times n_1} \quad \mathbf{Q}_{N \times 1}]$$

Example 3.1.1: Let $n_1 = 2$ with $s_1 = 3$ (levels: 1, 0, -1) and $s_2 = 4$ (levels: 3, 1, -1, -3) i.e. $3^2 \times 4$. The first three columns of \mathbf{X} corresponding to $\mathbf{X}_1, \mathbf{X}_2$ and \mathbf{X}_3 with $2(3^2 \times 4) = 72$ points are as follows:

$$\mathbf{X} = [\mathbf{O}_{72 \times 2} \quad \mathbf{Q}_{72 \times 1}]$$

$$\mathbf{o}_i = \mathbf{1}_{3^p \times 4} \otimes [1 \quad 0 \quad -1]' \otimes \mathbf{1}_{3^{2-i}}, p = i - 1, i = 1, 2.$$

$$\mathbf{q}_1 = \mathbf{1}_{3^2} \otimes [3 \quad 1 \quad -1 \quad -3]'$$

$$\mathbf{Q}_{72 \times 1} = [\mathbf{q}_1 \quad \mathbf{q}_1]'$$

The other columns of \mathbf{X} are generated as per model with 8 columns ($\mathbf{1}, \mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_1^2, \mathbf{X}_2^2, \mathbf{X}_3^2, \mathbf{X}_3^3$)

For $\alpha = 0.5$,

$$\mathbf{Z}'\mathbf{Z} = \begin{bmatrix} 288 & \mathbf{0}'_2 & 0 & 192\mathbf{1}'_2 & 1440 & 0 \\ & 66\mathbf{I}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 \\ & & 1296 & \mathbf{0}'_2 & 0 & 10512 \\ & & & \mathbf{A} & 960\mathbf{1}_2 & \mathbf{0}_2 \\ & & & & 11424 & 0 \\ & & & & & 92304 \end{bmatrix}$$

where $\mathbf{A} = 22\mathbf{I}_2 + 128\mathbf{J}_2$.

$$(\mathbf{Z}'\mathbf{Z})^{-1} = \begin{bmatrix} 0.05 & \mathbf{0}'_2 & 0 & -0.031'_2 & -0.001 & 0 \\ & 0.002\mathbf{I}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 \\ & & 0.01 & \mathbf{0}'_2 & 0 & -0.001 \\ & & & 0.04\mathbf{I}_2 & \mathbf{0}_2 & \mathbf{0}_2 \\ & & & & 0.002 & 0 \\ & & & & & 0.0001 \end{bmatrix}$$

Thus,

$$\begin{aligned} V(\hat{\beta}_0) &= 0.05\sigma^2, V(\hat{\beta}_1) = V(\hat{\beta}_2) = 0.02\sigma^2 \\ V(\hat{\beta}_3) &= 0.01\sigma^2, V(\hat{\beta}_{11}) = V(\hat{\beta}_{22}) = 0.04\sigma^2 \\ V(\hat{\beta}_{33}) &= 0.0002\sigma^2 \text{ and } V(\hat{\beta}_{333}) = 0.0001\sigma^2 \\ Cov(\hat{\beta}_0, \hat{\beta}_{11}) &= Cov(\hat{\beta}_0, \hat{\beta}_{22}) = -0.03\sigma^2, Cov(\hat{\beta}_0, \hat{\beta}_{33}) = -0.001\sigma^2 \end{aligned}$$

The variance of estimated response, $V(\hat{y}_0) = 0.056\sigma^2$ for all points in \mathbf{X} . Hence, the design is rotatable.

The method discussed in Section 3.1.1 leads to the following proposition:

Proposition 2: As the $V(\hat{y}_0)$ is the same for all points in \mathbf{X} which are equidistant from the design centre for $s_1^{n_1} \times s_2$ mixed-level factorial constructed as per the method given in 3.1.1, the design satisfies theorem 1 and hence rotatable.

For $\alpha = 0.5$, the eigen values of $(\mathbf{Z}'\mathbf{Z})^{-1}$ are 0.09, 0.04, 0.02, 0.02, 0.01, 0.005, 8.4×10^{-5} , 1×10^{-5} and D-efficiency of this design is 3.663. For $\alpha = 0.1$, D-efficiency of this design is 1.94.

3.1.2. For $n_2 = 0$ i.e., $s_1^{n_1}$

Consider n_1 factors having s_1 levels. The n_1 columns of \mathbf{X} corresponding to $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{n_1}$ of MLRDNE in $N = n_1 s_1^{n_1}$ points are developed as follows:

$$\mathbf{X} = [\mathbf{O}_{N \times n_1}]$$

The other columns of \mathbf{X} are generated as per the model and values of s_1 .

Example 3.1.2: Let $n_1 = 4$ with $s_1 = 3$ (levels: 1, 0, -1) i.e. 3^4 . The first four columns of \mathbf{X} corresponding to $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3$ and \mathbf{X}_4 and $4 \times 3^4 = 324$ points are as follows:

$$\mathbf{X} = [\mathbf{O}_{324 \times 4}]$$

The other columns of \mathbf{X} are generated as per the model with nine columns $(\mathbf{1}, \mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_4, \mathbf{X}_1^2, \mathbf{X}_2^2, \mathbf{X}_3^2, \mathbf{X}_4^2)$. For $\alpha = 0.3$,

$$\mathbf{Z}'\mathbf{Z} = \begin{bmatrix} 8.294 & \mathbf{0}'_4 & 552.96\mathbf{1}'_4 \\ & 380.34\mathbf{1}'_4 & \mathbf{O}_4 \\ & & \mathbf{B} \end{bmatrix}$$

where, $\mathbf{B} = 368.64\mathbf{J}_4 + 126.78\mathbf{I}_4$, \mathbf{I}_4 is identity matrix order 4×4 , \mathbf{J}_4 is matrix of 1's of order 4×4 , $\mathbf{1}_4$ is column vector of 1's of order 4×1 , \mathbf{O}_4 is a column vector

of 0's of order 4×1 and \mathbf{O}_4 is matrix of 0's of order 4×4 .

$$(\mathbf{Z}'\mathbf{Z})^{-1} = \begin{bmatrix} 0.015 & \mathbf{0}'_4 & -0.005\mathbf{1}'_4 \\ & 0.003\mathbf{1}'_4 & \mathbf{O}_4 \\ & & 0.008\mathbf{I}_4 \end{bmatrix}$$

The variance of estimated response, $V(\hat{y}_0) = 0.0152\sigma^2$ for all points in \mathbf{X} . Hence, the design is rotatable.

The method discussed in Section 3.1.2 leads to the following proposition:

Proposition 3: As the $V(\hat{y}_0)$ is the same for all points in \mathbf{X} which are equidistant from the design centre for $s_1^{n_1}$ mixed-level factorial constructed as per the method given in 3.1.2, the design satisfies theorem 1 and hence rotatable.

When $\alpha = 0.3$, the eigen values of $(\mathbf{Z}'\mathbf{Z})^{-1}$ are 0.02, 0.008, 0.008, 0.008, 0.003, 0.003, 0.003, 0.0004 and D-efficiency for this design is 0.785. If $\alpha = 0.8$, then D-efficiency of this design is 1.831.

4. $s_1^{n_1} \times s_2$ MLRDNE in Smaller Runs

The MLRDNE for $s_1^{n_1} \times s_2$ in a smaller number of runs can be obtained by taking $n_1 + 1$ columns of \mathbf{X} corresponding to $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{n_1+1}$ in $N = s_1^{n_1} \times s_2$ points are as follows:

$$\mathbf{X} = [\mathbf{C}_{N \times n_1} \quad \mathbf{d}]$$

where, $\mathbf{d} = (\text{column vector of } s_2 \text{ levels}) \otimes \mathbf{1}_{s_1^{n_1}}$

$$\mathbf{C}_{N \times n_1} = [\mathbf{c}_1 \quad \mathbf{c}_2 \quad \dots \quad \mathbf{c}_{n_1}]$$

$\mathbf{c}_i = \mathbf{1}_{s_1^j \times s_2} \otimes (\text{column vector of } s_1 \text{ levels}) \otimes \mathbf{1}_{s_1^{n_1-i}}$ where, $i = 1, \dots, n_1$ and $j = i - 1$. Each vector \mathbf{c}_i is of order $N \times 1$. The other columns of \mathbf{X} are generated as per the model and values of s_1 and s_2 .

Example 4.1: For $n_1 = 2$ with $s_1 = 3$ (levels: 1, 0, -1) and $s_2 = 4$ (levels: 3, 1, -1, -3) *i.e.* $3^2 \times 4$, the first three columns of \mathbf{X} corresponding to $\mathbf{X}_1, \mathbf{X}_2$ and \mathbf{X}_3 and $3^2 \times 4 = 36$ points are as follows:

$$\mathbf{X} = [\mathbf{C}_{36 \times 2} \quad \mathbf{d}]$$

where, $\mathbf{d} = [3 \quad 1 \quad -1 \quad -3]' \otimes \mathbf{1}_9$

$\mathbf{c}_i = \mathbf{1}_{3^j \times 4} \otimes [1 \quad 0 \quad -1]' \otimes \mathbf{1}_{3^{2-i}}$

The other columns of \mathbf{X} are generated as per the model with eight columns $(\mathbf{1}, \mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_1^2, \mathbf{X}_2^2, \mathbf{X}_3^2, \mathbf{X}_3^3)$ and for $\alpha = 0.7$,

$$\mathbf{Z}'\mathbf{Z} = \begin{bmatrix} 207.36 & 0 & 0 & 0 & 138.24 & 138.24 & 103.68 & 0 \\ & 81.12 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & 2.16 & 0 & 0 & 0 & 0 & 0 \\ & & & 922.56 & 0 & 0 & 0 & 7473.6 \\ & & & & 119.2 & 92.16 & 691.2 & 0 \\ & & & & & 92.88 & 691.2 & 0 \\ & & & & & & 8197.12 & 0 \\ & & & & & & & 65519.04 \end{bmatrix}$$

$$(\mathbf{Z}'\mathbf{Z})^{-1} = \begin{bmatrix} 0.64 & 0 & 0 & 0 & -0.025 & -0.93 & -0.002 & 0 \\ & 0.01 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & 0.46 & 0 & 0 & 0 & 0 & 0 \\ & & & 0.014 & 0 & 0 & 0 & -0.002 \\ & & & & 0.04 & 0 & 0 & 0 \\ & & & & & 1.39 & 0 & 0 \\ & & & & & & 0.0003 & 0 \\ & & & & & & & 0.0002 \end{bmatrix}$$

Variance of the estimated response, $V(\hat{y}_0) = 0.655\sigma^2$ for all points in \mathbf{X} and thus the design is rotatable. However, it can be seen that the variances of a particular order of estimates are not same unlike Example 3.1.1.

For $\alpha = 0.7$, the eigen values of $(\mathbf{Z}'\mathbf{Z})^{-1}$ are 2.015, 0.463, 0.051, 0.014, 0.012, 0.007, 0.0001, 0.00001 and this design having the D-efficiency 2.77. When $\alpha = 0.2$, D-efficiency of this design is 2.192.

A list of MLRDNE is given in Appendix 2 containing n_1, n_2, s_1, s_2 and the variance of estimated response at $\alpha = 0, 0.3, 0.5, 0.7$ and 0.9 . It is seen that in the presence of the neighbour effect and when the value of α increases, the variance of estimated response is in decreasing order.

5. R package for the Generation of MLRDNE

An R package named *rsdNE* has been developed for the generation of MLRDNE. It also computes the variance of parameter estimates and variance of the predicted response. The package is made available at <https://cran.r-project.org/package=rsdNE>. This package includes `sym()`, `asym1()`, `asym2()` functions that generates response surface designs which are rotatable under a polynomial model of a given order without interaction term incorporating neighbour effects. A few Snapshots of the package has been given in the Appendix 1.

6. Discussion

This article attempts to provide a series of rotatable response surface designs when immediate (left and right at distance 1) neighbour effects are suspected in an experiment. A general procedure for the construction of Mixed Level Rotatable Design with Neighbour Effects (MLRDNE) of the form $s_1^{n_1} \times s_2^{n_2}$ is given. For these designs it is seen that as the value of α increases the variance of the estimated response decreases and on the other hand, D-efficiency increases. The R package *rsdNE* developed would help the experimenter to generate MLRDNE design along with the variance of the parameter estimates as well as the variance of predicted response.

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Appendix 1

```

> library(rsdNE)
> asym1(1,1,0.5)
[1] "X matrix"
      [,1] [,2] [,3] [,4]
[1,]    1  -1  -1    1
[2,]    1   1   1    1
[3,]    1   1   0    0
[4,]    1   1  -1    1
[5,]    1  -1   1    1
[6,]    1  -1   0    0
[7,]    1  -1  -1    1
[8,]    1   1   1    1
[1] "Z_prime_Z matrix"
      [,1] [,2] [,3] [,4]
[1,]   24   0   0   16
[2,]    0  12   0   0
[3,]    0   0   1   0
[4,]   16   0   0   11
[1] "inv(Z_prime_Z) matrix"
      [,1] [,2] [,3] [,4]
[1,]  1.375 0.00000000  0  -2
[2,]  0.000 0.08333333  0   0
[3,]  0.000 0.00000000  1   0
[4,] -2.000 0.00000000  0   3
[1] "total number of runs" "6"
[1] "variance of estimated response" "1.4583"

```

Figure 1: 2 factors having 2 and 3 levels *i.e.* 2×3 when $\alpha = 0.5$

```

R 4.2.2 . ~/
> asym2(3,2,4,2,0.5)
      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11]
[1,]    1  -1  -1  -3  -3    1    1    9    9  -27  -27
[2,]    1   1   1   3   3    1    1    9    9   27   27
[3,]    1   1   0   3   1    1    0    9    1   27    1
[4,]    1   1  -1   3  -1    1    1    9    1   27  -1
[5,]    1   0   1   3  -3    0    1    9    9   27  -27
[6,]    1   0   0   1   3    0    0    1    9    1   27
[7,]    1   0  -1   1   1    0    1    1    1    1    1
[8,]    1  -1   1   1  -1    1    1    1    1    1  -1
[9,]    1  -1   0   1  -3    1    0    1    9    1  -27
[10,]   1  -1  -1  -1   3    1    1    1    9   -1   27
[11,]   1   1   1  -1   1    1    1    1    1   -1    1
[12,]   1   1   0  -1  -1    1    0    1    1   -1  -1
[13,]   1   1  -1  -1  -3    1    1    1    9   -1  -27
[14,]   1   0   1  -3   3    0    1    9    9  -27   27
[15,]   1   0   0  -3   1    0    0    9    1  -27    1
[16,]   1   0  -1  -3  -1    0    1    9    1  -27  -1
[17,]   1  -1   1  -3  -3    1    1    9    9  -27  -27
[18,]   1  -1   0   3   3    1    0    9    9   27   27
[19,]   1  -1  -1   3   1    1    1    9    1   27    1
[20,]   1   1   1   3  -1    1    1    9    1   27  -1
[21,]   1   1   0   3  -3    1    0    9    9   27  -27
[22,]   1   1  -1   1   3    1    1    1    9    1   27
[23,]   1   0   1   1   1    0    1    1    1    1    1

```

Figure 2: \mathbf{X} matrix for $3^2 \times 4^2$ MLRDNE

```
[1] "Z_prime_matrix"
      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11]
[1,] 1152    0    0    0    0  768  768  5760  5760    0    0
[2,]    0  264    0    0    0    0    0    0    0    0    0
[3,]    0    0  264    0    0    0    0    0    0    0    0
[4,]    0    0    0  2808    0    0    0    0    0  21816    0
[5,]    0    0    0    0  2808    0    0    0    0    0  21816
[6,]  768    0    0    0    0  600  512  3840  3840    0    0
[7,]  768    0    0    0    0  512  600  3840  3840    0    0
[8,]  5760    0    0    0    0  3840  3840  38592  28800    0    0
[9,]  5760    0    0    0    0  3840  3840  28800  38592    0    0
[10,]    0    0    0  21816    0    0    0    0    0  180792    0
[11,]    0    0    0    0  21816    0    0    0    0    0  180792
```

Figure 3: $\mathbf{Z}'\mathbf{Z}$ matrix for $3^2 \times 4^2$ MLRDNE

```
[1] "inv(Z_prime_Z) matrix"
      [,1] [,2] [,3] [,4] [,5] [,6]
[1,] 0.0160752748 0.000000000 0.000000000 0.000000000 0.000000000 -0.007575758
[2,] 0.000000000 0.003787879 0.000000000 0.000000000 0.000000000 0.000000000
[3,] 0.000000000 0.000000000 0.003787879 0.000000000 0.000000000 0.000000000
[4,] 0.000000000 0.000000000 0.000000000 0.0056985294 0.000000000 0.000000000
[5,] 0.000000000 0.000000000 0.000000000 0.000000000 0.0056985294 0.000000000
[6,] -0.0075757576 0.000000000 0.000000000 0.000000000 0.000000000 0.011363636
[7,] -0.0075757576 0.000000000 0.000000000 0.000000000 0.000000000 0.000000000
[8,] -0.0005106209 0.000000000 0.000000000 0.000000000 0.000000000 0.000000000
[9,] -0.0005106209 0.000000000 0.000000000 0.000000000 0.000000000 0.000000000
[10,] 0.000000000 0.000000000 0.000000000 -0.0006876362 0.000000000 0.000000000
[11,] 0.000000000 0.000000000 0.000000000 0.000000000 -0.0006876362 0.000000000
      [,7] [,8] [,9] [,10] [,11]
[1,] -0.007575758 -5.106209e-04 -0.0005106209 0.000000e+00 0.000000e+00
[2,] 0.000000000 0.000000e+00 0.000000000 0.000000e+00 0.000000e+00
[3,] 0.000000000 0.000000e+00 0.000000000 0.000000e+00 0.000000e+00
[4,] 0.000000000 0.000000e+00 0.000000000 -6.876362e-04 0.000000e+00
[5,] 0.000000000 0.000000e+00 0.000000000 0.000000e+00 -6.876362e-04
[6,] 0.000000000 0.000000e+00 0.000000000 0.000000e+00 0.000000e+00
[7,] 0.011363636 0.000000e+00 0.000000000 0.000000e+00 0.000000e+00
[8,] 0.000000000 1.021242e-04 0.000000000 0.000000e+00 0.000000e+00
[9,] 0.000000000 -2.834515e-20 0.0001021242 0.000000e+00 0.000000e+00
[10,] 0.000000000 0.000000e+00 0.000000000 8.850763e-05 0.000000e+00
[11,] 0.000000000 0.000000e+00 0.000000000 0.000000e+00 8.850763e-05
[1] "total number of runs" "288"
[1] "variance of estimated response" "0.0231"
>
```

Figure 4: $\mathbf{Z}'\mathbf{Z}^{-1}$ matrix, N and $V(\hat{y}_0)$ for $3^2 \times 4^2$ MLRDNE

Appendix 2

Table 3.1: MLRDNE

				$V(\hat{y}_0)$				
n_1	n_2	s_1	s_2	$\alpha = 0$	$\alpha = 0.3$	$\alpha = 0.5$	$\alpha = 0.7$	$\alpha = 0.9$
2	0	4	-	0.2188	0.1555	0.1166	0.0856	0.0638
2	0	5	-	0.1800	0.1212	0.0894	0.0653	0.0484
2	0	6	-	0.1528	0.0994	0.0723	0.0525	0.0390
2	1	2	4	0.2083	0.1663	0.1645	0.1361	0.0975
2	1	2	5	0.1750	0.1448	0.1395	0.1145	0.0822
2	1	2	6	0.1667	0.1304	0.1229	0.1002	0.0720
2	1	3	4	0.1111	0.0723	0.0556	0.0427	0.0330
2	1	3	5	0.1000	0.0625	0.0475	0.0363	0.0280
2	1	3	6	0.0926	0.0560	0.0422	0.0320	0.0246
2	1	4	2	0.1250	0.0844	0.0626	0.0458	0.0341
2	1	4	3	0.0937	0.0605	0.0445	0.0325	0.0241
2	1	4	5	0.0688	0.0414	0.0300	0.0218	0.0162
2	1	4	6	0.0625	0.0366	0.0263	0.0191	0.0142
2	1	5	2	0.1000	0.0647	0.0474	0.0345	0.0256
2	1	5	3	0.0733	0.0458	0.0333	0.0242	0.0179
2	1	5	4	0.0600	0.0364	0.0263	0.0190	0.0141
2	1	5	6	0.0467	0.0269	0.0192	0.0139	0.0103
2	1	6	2	0.0833	0.0525	0.0379	0.0275	0.0205
2	1	6	3	0.0602	0.0369	0.0265	0.0192	0.0142
2	1	6	4	0.0486	0.0290	0.0207	0.0150	0.0111
2	1	6	5	0.0417	0.0243	0.0173	0.0125	0.0093
2	2	2	5	0.0550	0.0476	0.0424	0.0336	0.0243
2	2	3	4	0.0382	0.0295	0.0231	0.0175	0.0134
2	2	3	5	0.0289	0.0213	0.0164	0.0124	0.0094
2	2	4	5	0.0188	0.0133	0.0099	0.0073	0.0054
2	2	5	6	0.0106	0.0071	0.0052	0.0038	0.0028