Evaluation of the Block Effects in Response Surface Designs with Random Block Effects over Cuboidal Regions

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Abstract

In many experimental situations, whenever a block design is used, the block effect is usually considered to be fixed. There are, however, experimental situations in which it should be treated as random. The choice of a blocking arrangement for a response surface design can have a considerable effect on estimating the mean response and on the size of the prediction variance even if the experimental runs are the same. Therefore, care should be exercised in the selection of blocks. In this paper, in the presence of a random block effect, we propose a graphical method for evaluating the effect of blocking in response surface designs using cuboidal regions. This graphical method can be used to investigate how the blocking has influence on the prediction variance throughout all experimental regions of interest when this region is cuboidal, and compare the block effects in the cases of the orthogonal and non-orthogonal block designs, respectively.

Keywords: response surface design; random block effect; cuboidal region moment; blocking effect graph.

1. Introduction

The traditional method in most response surface applications is to treat the block effect as fixed in the assumed model. There are, however, experimental situations in which it is more appropriate to consider the block effect as random. It is important to properly identify the nature of the block effect since the type of analysis to be used depends on whether the block effect is fixed or random. Consequently, doing a fixed-effects analysis instead of a random-effects analysis when the block effect is random may, in general, lead to incorrect conclusions. In general, random effects occur as a result of sampling from large population. The presence of random block effects, in addition to the usual fixed polynomial effects, in a response surface model results in a so-called mixed model. The use of such a model in a response surface environment was first considered by Khuri(1992), and Khuri(1996) extended

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his work by the addition of interaction terms between the fixed polynomial effects and the random block effects.

The conditions for a response surface design to block orthogonally were given by Box and Hunter(1957) for a second-order model and by Khuri(1992) for the general case of a model of order $d(\ge 1)$. In many experimental situations, a response surface design may not block orthogonally. Therefore, it is imperative that the block effect be accounted for before any exploration of the response surface is carried out. Dey and Das(1970) introduced the concept of non-orthogonal blocking for the special case of second order models and Adhikary and Panda(1990) presented a sequential method for constructing second-order rotatable designs in non-orthogonal blocks. More recently, Khuri(1994) demonstrated the effects of the blocks on estimating the mean response, on the prediction variance and on the optimum of the response surface model with fixed block effects.

As a graphical technique for evaluating the prediction capability of response surface designs, Giovannitti-Jensen and Myers(1989) proposed a variance-based graphical approach for standard response surface designs that considers plots of the maximum, the minimum and the spherical average of the prediction variance on spheres of varying radii inside a region of interest. In addition to the prediction variance, Vining and Myers(1991) extended a graphical procedure for evaluating response surface designs in terms of the mean squared error of prediction and as another graphical method for evaluating the prediction capability of response surface designs, Khuri, Kim and Um(1996) proposed quantile plots of the prediction variance for response surface designs. Using the concepts of Khuri(1992, 1994) and Giovannitti-Jensen and Myers(1989), in the presence of a fixed block effect, Park and Jang(1999a) proposed measures for evaluating the effect of blocking in response surface designs in terms of prediction variance when a region of interest is spherical. And Park and Jang(1999b) proposed another graphical method for evaluating the effect of blocking in response surface designs.

All of the discussion and illustration in the preceding papers deals with prediction variance for spherical regions. In this case it is natural to observe values of prediction variance(apart from random error variance) averaging over the volumes or surfaces of spheres. However, it is not natural to deal with the volumes or surfaces of spheres when the natural region of interest is a cube(See Myers and Montgomery(1995, p.381).). Rozum and Myers(1991) and Myers et al.(1992) extended the work of Giovannitti-Jensen and Myers(1989) from spherical to cuboidal regions. Both are useful tools for comparing competing designs or blocking arrangements of a response surface design. Using the ideas proposed by Khuri(1994) and Rozum and Myers(1991), Park and Jang(1998) proposed a graphical method for evaluating the effect of blocking in response surface designs using cuboidal regions in the presence of a fixed block effect, and Park and Jang(1999c) proposed a measure for evaluating the effect of blocking in response surface designs using cuboidal regions in the cases of fixed effects and random effects, respectively. The drawback of the measures proposed by Park and Jang(1999a,c) gives only single-valued criteria for the entire experimental region, but the

above-mentioned graphical method describes what happens inside a region of interest, R and provides better comparisons among blocking arrangements.

In this paper, using the ideas proposed by Khuri(1992), Rozum and Myers(1991) and Giovannitti-Jensen and Myers(1989), we propose a graphical method for evaluating the effect of blocking in response surface designs with random block effects over cuboidal regions. This article will be the extended work of Park and Jang(1998). This graphical method can be used to assess graphically the overall variation in the prediction variance resulting from blocking, throughout the entire experimental regions of interest, when this region is cuboidal, and compare the block effects in the cases of the orthogonal and non-orthogonal block designs, respectively.

2. The Effect of Blocking on the Prediction Variance in Model with Random Block Effects

Let us consider a response surface model of order $d(\ge 1)$ in k input variables, x_1, x_2, \dots, x_k . The mean response, $\eta(\underline{x})$, at a point $\underline{x} = (x_1, x_2, \dots, x_k)'$ inside a region of interest R is given as

$$\eta(x) = x_{\beta}' \beta \tag{1}$$

where $x_{\beta}' = (1, x_1, x_2, \cdots, x_p)$ is a vector of order $1 \times (p+1)$ whose elements consist of the x_i terms along with their powers and cross-products of these powers up to a degree d and $\beta = (\beta_0, \beta_1, \beta_2, \cdots, \beta_p)'$ is the vector of unknown constant parameters. For a first order model $x_{\beta}' = (1, x_1, x_2, \cdots, x_k)$ and $\beta = (\beta_0, \beta_1, \beta_2, \cdots, \beta_k)'$ and for a second order model $x_{\beta}' = (1, x_1, x_2, \cdots, x_k, x_1^2, x_2^2, \cdots, x_k^2, x_1x_2, \cdots, x_1x_k, \cdots, x_{k-1}x_k)$ and $\beta = (\beta_0, \beta_1, \beta_2, \cdots, \beta_k, \beta_{11}, \beta_{22}, \cdots, \beta_{kk}, \beta_{12}, \cdots, \beta_{k-1k})'$.

Suppose that the experimental runs used to fit a response surface model are not homogeneous due to the presence of an extraneous source of variation, denoted by δ , whose levels is a random sample from a much larger population. Let the experimental runs be arranged in b blocks, where the runs within a block are somewhat homogeneous and n_j denote the size of the jth block($j=1,2,\cdots,b$) such that $n=\sum_{j=1}^b n_j$. The response vector \underline{y} which consists of the n observations, can then be represented by the model

$$y = X \beta + Z \delta + \varepsilon \tag{2}$$

where X is an $n \times (p+1)$ model matrix, the elements of the vector $\underline{\beta} = (\beta_0, \beta_1, \beta_2, \dots, \beta_p)'$ are unknown constant parameters, $\underline{\delta} = (\delta_1, \delta_2, \dots, \delta_b)'$, where δ_j denotes the effect of the jth block, Z is a block-diagonal matrix of form $Z = diag(1_{n_1}, 1_{n_2}, \dots, 1_{n_b})$, where 1_{n_j} is a

vector of ones of order $n_j \times 1$ $(j=1,2,\dots,b)$ and $\underline{\varepsilon}$ is the $n \times 1$ vector of random errors which is assumed to have a zero mean and a variance-covariance matrix $\sigma_{\varepsilon}^2 I_n$, where I_n is the identity matrix of order $n \times n$.

Unlike the case of a fixed block effect, this case deals with situations in which the block effect in model (2) is random so that $\underline{\delta}$ is distributed as $(0, \sigma_{\delta}^2 I_b)$ independently of $\underline{\varepsilon}$. Model (2) is therefore a mixed model, since $\underline{\beta}$ is a fixed parameter vector. The mean response vector and variance-covariance matrix of \underline{y} are respectively $E(\underline{y}) = X \underline{\beta}$ and

$$\sum = \sigma_{\varepsilon}^2 I_n + \sigma_{\delta}^2 Z Z' = \sigma_{\varepsilon}^2 A \tag{3}$$

where $A = diag(A_1, A_2, \dots, A_b)$, where $A_j = I_{n_j} + \zeta J_{n_j}$, $(j = 1, 2, \dots, b)$, where J_{n_j} is an $n_j \times n_j$ matrix of ones and

$$\zeta = \sigma_0^2 / \sigma_{\varepsilon}^2. \tag{4}$$

In general, ζ is unknown and should therefore be estimated by finding suitable estimates of the variance components, σ_{δ}^2 and σ_{ε}^2 . However, since our concerns is merely in the performance of an experimental design, we consider a fixed ratio ζ . Khuri(1992) demonstrated that if the ratio ζ is known, then the BLUE of β is the generalized least squares estimator $\widehat{\beta}_{\varepsilon}$ given by $\widehat{\beta}_{\varepsilon} = (X'A^{-1}X)^{-1}X'A^{-1}y$ and the variance-covariance matrix of $\widehat{\beta}_{\varepsilon}$ is

$$Var(\widehat{\beta}_g) = (X'A^{-1}X)^{-1}\sigma_{\varepsilon}^2.$$
 (5)

And the predicted value of the mean response in model (1) is given by

$$\widehat{\eta_g}(\underline{x}) = \underline{x_\beta}' \widehat{\beta_g}. \tag{6}$$

The prediction variance of $\widehat{\eta_g}(x)$ can therefore be written as

$$Var[\widehat{\eta_{\varepsilon}}(\underline{x})] = \underline{x_{\theta}}'(X'A^{-1}X)^{-1}\underline{x_{\theta}}\sigma_{\varepsilon}^{2}. \tag{7}$$

It is meaningful to compare the prediction variances of a blocked design and an unblocked design when there are block effects, that is, $\sigma_{\delta}^2 > 0$. Though there are block effects, the ordinary least-squares estimator $\widehat{\mathcal{B}}_o$ of \mathcal{B} obtained by ignoring the block effects is used as $\widehat{\mathcal{B}}_o = (X'X)^{-1}X'y$ and the variance-covariance matrix of $\widehat{\mathcal{B}}_o$ is

$$Var(\widehat{\beta}_0) = (X'X)^{-1}X'AX(X'X)^{-1}\sigma_{\epsilon}^2.$$
 (8)

And the predicted value of the mean response in model (1) is given by

$$\widehat{\eta_o}(\underline{x}) = \underline{x_{\beta}}' \widehat{\underline{\beta}_o}.$$

The prediction variance of $\widehat{\eta}_o(\underline{x})$ can therefore be written as

$$Var[\widehat{\eta_o}(x)] = x_{\beta}'(X'X)^{-1}X'AX(X'X)^{-1}x_{\beta}\sigma_{\varepsilon}^2.$$
(9)

Note that in a standard response surface model with no random effects, $\widehat{\beta}_g = \widehat{\beta}_o = \widehat{\beta} = \widehat{\beta}_o$

$$(X'X)^{-1}X'y$$
, $Var(\widehat{\beta}_g) = Var(\widehat{\beta}_o) = Var(\widehat{\beta}) = (X'X)^{-1}\sigma_{\varepsilon}^2$, and hence
$$Var[\widehat{\eta_{\varepsilon}}(x)] = Var[\widehat{\eta_{\varepsilon}}(x)] = Var[\widehat{\eta_{\varepsilon}}(x)],$$

where $Var[\hat{\eta}_0(x)]$ denotes the prediction variance when the block effects are zero.

3. A Graphical Method for Evaluating the Effect of Blocking in Response Surface Designs

All of the discussions and illustrations in the above-mentioned papers deal with prediction variance when a region of interest is spherical. However, it is not natural to deal with the volumes or surfaces of spheres when the natural region of interest is a cube. That is, cubes nested inside the design cube can be more natural. Rozum and Myers(1991) extended the work of Giovannitti-Jensen and Myers(1989) from spherical to cuboidal regions. In the presence of a fixed block effect, Park and Jang(1998) proposed a graphical method for evaluating the effect of blocking in response surface designs using cuboidal regions. Park and Jang(1999c) proposed a numeric measure for evaluating the effect of blocking in response surface designs using cuboidal regions in the cases of fixed effects and random effects, respectively.

Thus, so as to assess graphically the overall variation in the prediction variance caused by blocking, throughout the entire experimental regions of interest, we propose a graphical method that quantifies the effect of blocking in response surface designs with a random block effect over cuboidal regions. From the formulas (7) and (9), let us consider

$$V_B(x) = \frac{Var[\widehat{\eta_g}(x)]}{\sigma_{\varepsilon}^2} = x_{\beta}'(X'A^{-1}X)^{-1}x_{\beta}$$
 (10)

and

$$V_{U}(\underline{x}) = \frac{Var[\widehat{\eta_{o}}(\underline{x})]}{\sigma_{\varepsilon}^{2}} = \underline{x_{\beta}}'(X'X)^{-1}X'AX(X'X)^{-1}\underline{x_{\beta}}. \tag{11}$$

From the formulas (10) and (11), we define quantities as followings;

$$CV_{avg}^{B}(r) = \psi \int_{C_{r}} V_{B}(x) dx$$

$$= \psi \int_{C_{r}} x_{\beta}' Q_{B} x_{\beta} dx$$
(12)

is called the cuboidal average blocking variance and

$$CV_{avg}^{U}(r) = \psi \int_{C_{r}} V_{U}(x) dx$$

$$= \psi \int_{C_{r}} x_{\beta}' Q_{U} x_{\beta} dx$$
(13)

is called the cuboidal average unblocking variance. Here, the radius r is defined as the distance from the center of the hypercube to its face, C_r is the surface of a hypercube with

a radius r defined by $C_r = \{\underline{x}: -r \leq x_i \leq r, i=1,2,\cdots,k; i \neq j; x_j = \pm r\}, \quad \psi^{-1} = \int_{C_r} d\underline{x}$ implies integration over the surface of the hypercube with a radius r and Q_B is the matrix of order $(p+1)\times(p+1)$ of the form $Q_B = (X'A^{-1}X)^{-1}$ and Q_U is the matrix of order $(p+1)\times(p+1)$ of the form $Q_U = (X'X)^{-1}X'AX(X'X)^{-1}$ and $\psi^{-1} = \int_{C_r} d\underline{x}$ is the surface area of C_r . By applying the properties of the trace, $CV_{avg}^B(r)$ and $CV_{avg}^U(r)$ are written by

$$CV_{avg}^{B}(r) = \psi \int_{C_{r}} tr[X_{\beta}' Q_{B} X_{\beta}] dX$$

$$= tr[\psi \int_{C_{r}} X_{\beta} X_{\beta}' Q_{B} dX]$$

$$= tr[C^{*}Q_{B}]$$
(14)

and

$$CV_{avg}^{U}(r) = \psi \int_{C_{r}} tr[X_{\beta}' Q_{U} X_{\beta}] dX$$

$$= tr[\psi \int_{C_{r}} X_{\beta} X_{\beta}' Q_{U} dX]$$

$$= tr[C^{*}Q_{U}]$$
(15)

where $C^* = \psi \int_{C_r} x_\beta \ x_{\beta'} dx$ is the matrix of the cuboidal region moments, the region being the hypercube defined by C_r .

Rozum and Myers(1991) derived the following cuboidal region moments for the case where C_r is the surface of a hypercube with face of length 2r defined by $C_r = \{\underline{x} : -r \leq x_i \leq r, i = 1, 2, \dots, k; i \neq j; x_j = \pm r\}$. Let

$$\psi^{-1} = \int_{C_r} dx = \sum_{j=1}^k \left[\int_{-r}^r \cdots \int_{-r}^r dx_1 \cdots dx_{j-1} dx_{j+1} \cdots dx_k + \int_{-r}^r \cdots \int_{-r}^r dx_1 \cdots dx_{j-1} dx_{j+1} \cdots dx_k \right],$$

where the first multiple integral is on the hypercube with $x_j = -r$ and the second multiple integral is on the hypercube with $x_j = r$. Then, a cuboidal region moment of order q on C_r is defined as following;

$$\sigma_{q_{1}q_{2}\cdots q_{s}} = \psi \int_{C_{r}} x_{1}^{q_{1}} x_{2}^{q_{2}} \cdots x_{k}^{q_{s}} dx$$

$$= 2\psi \sum_{i=1}^{k} \int_{-r}^{r} \cdots \int_{-r}^{r} x_{1}^{q_{1}} x_{2}^{q_{2}} \cdots x_{k}^{q_{s}} dx_{1} \cdots dx_{j-1} dx_{j+1} \cdots dx_{k}$$
(16)

where $\phi^{-1} = \int_{C_r} d\underline{x} = k2^k r^{k-1}$ is the surface area of C_r with a radius r and q_1, q_2, \cdots, q_k are nonnegative integers such that $\sum_{i=1}^k q_i = q \le 2d$. Since C_r is a symmetric region, the cuboidal region moment $\sigma_{q_1q_2\cdots q_k}$ is 0 if at least one q_i is odd $(i=1,2,\cdots,k)$. The cuboidal region

moments that are used in the development of a graphical method for the first-order and second-order model cases are the second and fourth-order cuboidal region moments given by

$$\sigma_{2} = \psi \int_{C_{r}} x_{i}^{2} dx = \frac{(k+2)r^{2}}{3k} ,$$

$$\sigma_{4} = \psi \int_{C_{r}} x_{i}^{4} dx = \frac{(k+4)r^{4}}{5k} ,$$

$$\sigma_{22} = \psi \int_{C_{r}} x_{i}^{2} x_{i}^{2} dx = \frac{(k+4)r^{4}}{9k} .$$
(17)

Thus, by applying the cuboidal region moments in the formulas (16) and (17) to the formulas (14) and (15), we obtain that in the case of a first-order model,

$$CV_{avg}^{B}(r) = d^{00} + \frac{(k+2)r^2}{3k} \sum_{i=1}^{k} d^{ii}$$

and

$$CV_{avg}^{U}(r) = e^{00} + \frac{(k+2)r^2}{3k} \sum_{i=1}^{k} e^{ii}$$

and that in the case of a second-order model,

$$CV_{avg}^{B}(r) = d^{00} + \frac{(k+2)r^{2}}{3k} \left(\sum_{i=1}^{k} d^{ii} + 2 \sum_{i=k+1}^{2k} d^{1i} \right) + \frac{(k+4)r^{4}}{k} \left(\frac{1}{5} \sum_{i=k+1}^{2k} d^{ii} + \frac{1}{9} \left(\sum_{i=2k+1}^{b} d^{ii} + \sum_{i=k+1}^{2k} \sum_{\substack{j=k+1\\j \neq i}}^{2k} d^{ij} \right) \right)$$
(18)

and

$$CV_{avg}^{U}(r) = e^{00} + \frac{(k+2)r^{2}}{3k} \left(\sum_{i=1}^{k} e^{ii} + 2 \sum_{i=k+1}^{2k} e^{1i} \right) + \frac{(k+4)r^{4}}{k} \left\{ \frac{1}{5} \sum_{i=k+1}^{2k} e^{ii} + \frac{1}{9} \left(\sum_{i=2k+1}^{k} e^{ii} + \sum_{i=k+1}^{2k} \sum_{\substack{j=k+1\\i\neq j}}^{2k} e^{ij} \right) \right\}$$

$$(19)$$

where d^{ij} is the (ij) element of Q_B and e^{ij} is the (ij) element of Q_U $(i,j=0,1,2,\cdots,p)$. The quantity, $CV_{avg}^B(r)$, is the average of the prediction variances after blocking throughout the entire experimental regions on the surface of the hypercube with a radius r, and hence appears as a function of r. The quantity, $CV_{avg}^U(r)$, is the average of the prediction variances obtained by ignoring block effects throughout the entire experimental regions on the surface of the hypercube with a radius r when there are block effects, and hence appears as a function of r.

Also, from the formulas (10) and (11), let us consider

$$CV_{\max}^{B}(r) = \max_{\mathbf{x} \in C_{r}} [x_{\beta}' Q_{B} x_{\beta}]$$

$$CV_{\min}^{B}(r) = \min_{\mathbf{x} \in C_{r}} [x_{\beta}' Q_{B} x_{\beta}]$$
(20)

and

$$CV_{\max}^{U}(r) = \max_{x \in C_{r}} [x_{\beta}' Q_{U} x_{\beta}]$$

$$CV_{\min}^{U}(r) = \min_{x \in C_{r}} [x_{\beta}' Q_{U} x_{\beta}]$$
(21)

where $C_r = \{\underline{x}: -r \leq x_i \leq r, i=1,2,\cdots,k; i\neq j; x_j = \pm r\}$, $Q_B = (X'A^{-1}X)^{-1}$ and $Q_U = (X'X)^{-1}X'AX(X'X)^{-1}$. Then, it is required that these quantities, $CV_{\max}^B(r)$, $CV_{\min}^B(r)$, $CV_{\max}^U(r)$ and $CV_{\min}^U(r)$ be maximized and minimized over locations on a hypercube with a radius r. These quantities can be used as a graphical method to assess graphically the overall variation in the prediction variance resulting from blocking, throughout the entire experimental regions of interest, when this region is cuboidal. Thus, we can plot these quantities, $CV_{\max}^B(r)$, $CV_{\max}^B(r)$, $CV_{\min}^B(r)$, $CV_{\max}^U(r)$, $CV_{\max}^U(r)$ and $CV_{\min}^U(r)$, against a radius r. We call this graph the blocking effect graph(BEG) in the case of a random block effect when a region of interest is cuboidal.

Through these graphs, we can investigate more clearly the overall variation of the prediction variances caused by blocking against a radius r and compare the block effects in the cases of the orthogonal and non-orthogonal block designs, respectively, and hence we can clearly see that to choose which blocking arrangement in the same experimental runs with a random block effect is more effective in terms of prediction variance when this region is cuboidal.

4. A Numerical Example

Let us consider the example used in Khuri(1994) and Park and Jang(1998, 1999a,b,c). This example is based on an experiment described by Box and Draper (1987, p.360), concerning a small reactor study. The experiment was performed sequentially in four blocks, each consisting of six runs. Three input variables were considered (i.e. F: flow rate in liters per hour, C: concentration of catalyst, T: temperature). Table 1 shows the basic design described by Box and Draper (1987). A second-order model in x_1 , x_2 and x_3 was fitted. Here, x_1 , x_2 and x_3 denote the coded values of F, C and T, respectively. The basic design is of the central composite form with four center points and a replicated axial portion. This particular design is rotatable and blocks orthogonally, as can be verified by applying Box and Hunter's(1957) conditions.

In order to illustrate the effect of blocking on prediction variance, let us consider other blocking arrangements of the same 24 experimental runs in Table 1. These blocking arrangements are described in Table 2 which is modified from Table 2 in Khuri(1994), which are the same blocking arrangements used in Park and Jang(1999a,c). All blocking arrangements are scaled so that the design perimeter is restricted to being inside a unit cube.

Table 1. The basic design

Block	Exp. run	x_1	x_2	x_3	
1	1 2 3 4 5 6	-1 1 -1 1 0 0	-1 -1 1 1 0 0	1 -1 -1 1 0 0	
2	7 8 9 10 11 12	-1 1 -1 1 0 0	-1 -1 1 0 0	-1 1 1 -1 0 0	
3	13 14 15 16 17 18	$ -\sqrt{2} \\ \sqrt{2} \\ 0 \\ 0 \\ 0 \\ 0 $	$\begin{array}{c} 0 \\ 0 \\ -\sqrt{2} \\ \sqrt{2} \\ 0 \\ 0 \end{array}$	$\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ -\sqrt{2} \\ \sqrt{2} \end{array}$	
4	19 20 21 22 23 24	$ -\sqrt{2} \\ \sqrt{2} \\ 0 \\ 0 \\ 0 \\ 0 $	$ \begin{array}{c} 0 \\ 0 \\ -\sqrt{2} \\ \sqrt{2} \\ 0 \\ 0 \end{array} $	$ \begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ -\sqrt{2} \\ \sqrt{2} \end{array} $	

Unlike the case of a fixed block effect, in this case of a random block effect, it must be considered the value of the ratio $\zeta = \sigma_{\delta}^2/\sigma_{\epsilon}^2$. In general, the ratio ζ is unknown and should therefore be estimated from the data. However, since our concerns is merely in the performance of an experimental design, according to the various values of ζ with an appropriate size $(\zeta = 0 \sim 1.0)$, computations are made of the maximum, the minimum and the cuboidal average of prediction variances – $CV_{\max}^B(r)$, $CV_{\min}^B(r)$, $CV_{\max}^B(r)$, $CV_{\max}^U(r)$, $CV_{\min}^U(r)$ and $CV_{avg}^U(r)$ – resulting from blocking and unblocking, respectively, for the basic design and several blocking arrangements described in Table 2. We have tried to depict the blocking effect graphs for several blocking arrangements against varying ζ . As the results, we have found that these quantities for each blocking arrangement increase gradually as ζ increases and these quantities resulting from unblocking for each blocking arrangement are always greater than or equal to those resulting from blocking. That is, $Var[\widehat{\eta_{\theta}}(x)] \ge Var[\widehat{\eta_{\theta}}(x)]$

against varying ζ in the presence of a random block effect. This result is opposite to the case of a fixed block effect. Thus, we shall consider only in the case of a fixed $\zeta = 0.5$, because it has revealed to have a similar tendency for all the values of ζ .

Table 2. Division of the experimental runs described in Table 1 for the blocking arrangements

for the blocking drangoments						
Blocking arrangement	Block 1	Block 2	Block 3	Block 4		
1	1, 2, 5	3, 4, 7	13,14,15	19,20,21		
	6,11,12	8, 9, 10	16,17,18	22,23,24		
2	3, 4, 5	9,10,11	1, 2, 15	7, 8, 21		
	6,13,14	12,19,20	16,17,18	22,23,24		
3	2, 3, 4	8, 9, 10	1,14,15	7,20,21		
	5, 6,13	11,12,19	16,17,18	22,23,24		
4	1, 2, 3	7, 8, 9	6,14,15	12,20,21		
	4, 5,13	10,11,19	16,17,18	22,23,24		
5	3, 4, 5	7, 8, 9	1, 2,15	19,20,21		
	6,13,14	10,11,12	16,17,18	22,23,24		
6	1, 2, 3, 4 5, 6, 7, 8 9,10,11,12	13,14,15 16,17,18	19,20,21 22,23,24			

It should be noted that blocking arrangement 6 is orthogonal, as can be verified by applying Box and Hunter's(1957) conditions. But the other blocking arrangements are not orthogonal. It also should be noted that blocking arrangement $1 \sim 5$ have the same number of blocks and the same block sizes as in the basic design, but the allocation of experimental runs to the blocks is not the same. Figure $1 \sim 7$ show the blocking effect graphs for several blocking arrangements with a random effect against a radius r in a cuboidal region when $\zeta = 0.5$. The BEGs show the dispersion in the prediction variances resulting from blocking and unblocking, respectively, as a radius r increases. From these Figures, we can clearly see the overall change of the block effects for each blocking arrangement as a radius r varies. On the whole, the BEGs of all blocking arrangements show serious dispersion as r moves beyond about 0.6, particularly at the design perimeter and each quantity resulting from

unblocking is always greater than or equal to that resulting from blocking.

From Figure 1, the BEG for the basic design shows that each quantity – the maximum, the minimum and the cuboidal average of the prediction variances resulting from blocking and unblocking, respectively – is same as a radius r increases. This means that for this basic design, blocking causes no change in the prediction variance. But unlike in the case of a spherical region, their dispersions occur seriously as r proceeds towards the design perimeter. From Figure 7, we can find that though blocking arrangement 6 is orthogonal, each quantity for this blocking arrangement is not same because of the different block sizes as a radius r increases.

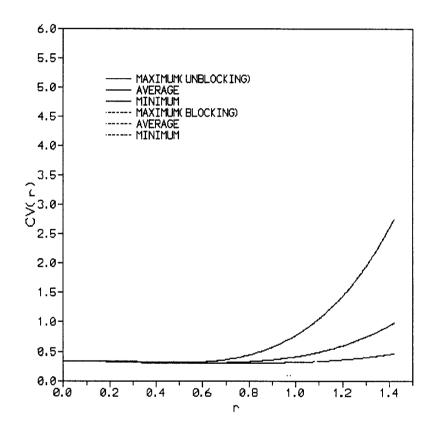


Figure 1. Blocking effect graph for the basic design with a random effect against a radius r in a cuboidal region ($\xi = 0.5$)

From Figure $2 \sim 6$, comparing the non-orthogonal blocking arrangements $1 \sim 5$ which have the same number of blocks and block sizes, we can see that none of all blocking arrangements show dispersion near the design center, and blocking arrangement 4 minimizes the overall change in the prediction variance throughout all experimental region. That is, we can find the fact that blocking arrangement 4 is more effective than the others in terms of

prediction variance.

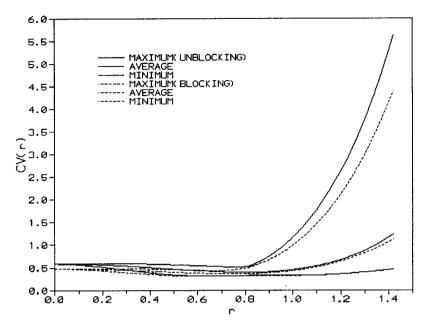


Figure 2. Blocking effect graph for blocking arrangement 1 with a random effect against a radius r in a cuboidal region ($\zeta = 0.5$)

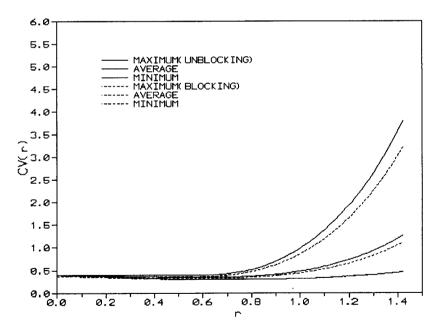


Figure 3. Blocking effect graph for blocking arrangement 2 with a random effect against a radius r in a cuboidal region (ζ =0.5)

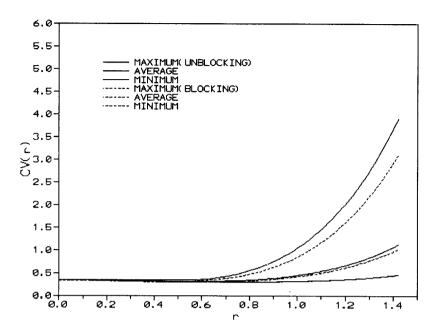


Figure 4. Blocking effect graph for blocking arrangement 3 with a random effect against a radius r in a cuboidal region ($\zeta = 0.5$)

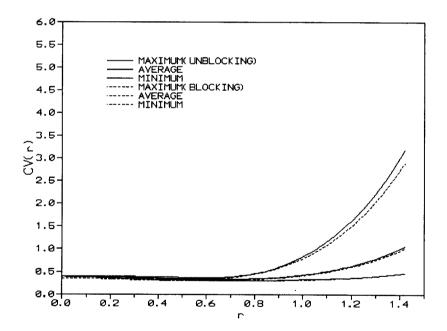


Figure 5. Blocking effect graph for blocking arrangement 4 with a random effect against a radius r in a cuboidal region ($\zeta = 0.5$)

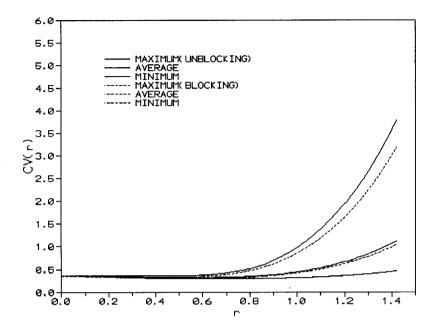


Figure 6. Blocking effect graph for blocking arrangement 5 with a random effect against a radius $\, r \,$ in a cuboidal region ($\, \zeta = 0.5 \,$)

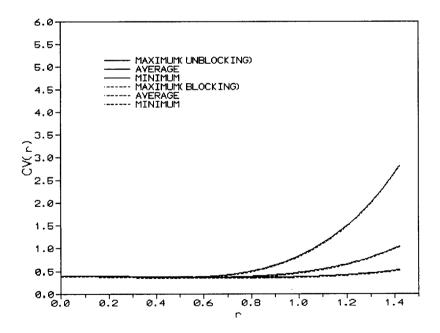


Figure 7. Blocking effect graph for blocking arrangement 6 with a random effect against a radius r in a cuboidal region (ζ =0.5)

Figure 8 shows the graph of differences between the cuboidal average unblocking variances and the cuboidal average blocking variances for several blocking arrangements with a random effect against the radius r in a cuboidal region (ζ =0.5). Comparing the BEGs of the basic design and blocking arrangements 6 which are orthogonal, we can see that the BEGs of these two blocking arrangements appear to be in a straight line which have the constant values as a radius r increases, and particularly the difference for the basic design is zero as a radius r increases. This means that for this basic design, blocking causes no change in the prediction variance at all points of the experimental region. But we find that though blocking arrangement 6 is orthogonal, the difference for this blocking arrangement is not zero because of the different block sizes. From Figure 8, we can also find that the BEG for blocking arrangement 1 appears to be highest at the center of the design region.

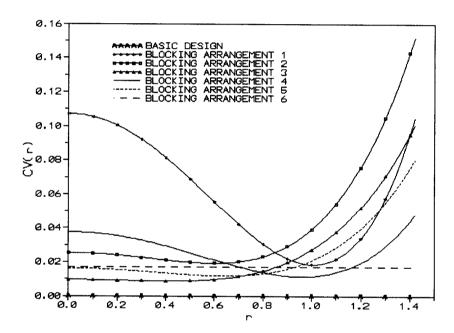


Figure 8. Graph of differences the cuboidal average unblocking variances and the cuboidal average blocking variances for several blocking arrangements with a random effect against a radius r in a cuboidal region ($\zeta = 0.5$)

5. Conclusions

In this paper, a graphical method has been proposed that allows us to evaluate the effect of blocking in response surface designs with random block effects over cuboidal regions. The proposed graphical method can be used as a useful tool for evaluating the effect of blocking in response surface designs with a random effect in terms of prediction variance when a region of interest is cuboidal. That is, in the presence of a random block effect, through the blocking effect graph, we can investigate more clearly the overall variation of the prediction variances throughout the entire experimental regions of interest when this region is cuboidal, and compare the block effects in the cases of the orthogonal and non-orthogonal block designs, respectively, and hence we can clearly see that to choose which blocking arrangement in the same experimental runs with a random block effect is most effective in terms of prediction variance when a region of interest is cuboidal.

As the extension of this paper in addition to the prediction variance, it is also interesting to depict the design's performance over the region of interest on bias to model misspecification.

References

- [1] Adhikary, B. and Panda, R.(1990), "Sequential Method of Conducting Rotatable Designs", Sankhyá, Series B, Vol. 52, pp. 212-218.
- [2] Box, G. E. P. and Draper, N. R.(1987), *Empirical Model-Building and Response Surfaces*, John Wiley & Sons, Inc., New York.
- [3] Box, G. E. P. and Hunter, J. S.(1957), "Multi-factor Experimental Designs for Exploring Response Surfaces", *The Annals of Mathematical Statistics*, Vol. 28, pp. 195-241.
- [4] Dey, A. and Das, M. N.(1970), On Blocking Second Order Rotatable Designs, Calcutta Statistical Association Bulletin, Vol. 19, pp. 75-85.
- [5] Giovannitti-Jensen, A. and Myers, R. H.(1989), "Graphical Assessment of the Prediction Capability of Response Surface Designs", *Technometrics*, Vol. 31, pp. 159-172.
- [6] Khuri, A. I.(1992), "Response Surface Models with Random Block Effects", Technometrics, Vol. 34, pp. 26-37.

- [9] Khuri, A. I., Kim, H. J. and Um, Y. H.(1996), "Quantile plots of the Prediction Variance for Response Surface Designs", Computational Statistics & Data Analysis, Vol. 22, pp. 395-407.
- [10] Myers, R. H. and Montgomery, D. C.(1995), *Response Surface Methodology*, John Wiley & Sons, Inc., New York.
- [11] Myers, R. H., Vining, G. G. and Giovannitti-Jensen, A.(1992), "Variance Dispersion Properties of Second-Order Response Surface Designs", *Journal of Quality Technology*, Vol. 24, pp. 1-11.

- [12] Park, S. H. and Jang, D. H.(1998), "A Graphical Method for Evaluating the Effect of Blocking in Response Surface Designs Using Cuboidal Regions", *The Korean Communications in Statistics*, Vol. 5, No. 3, 607-621.

- [16] Rozum, M. A. and Myers, R. H.(1991), "Variance Dispersion Graphs for Cuboidal Regions", paper presented at ASA Meetings, Atlanta, GA.
- [17] Vining, G. G. and Myers, R. H.(1991). "A Graphical Approach for Evaluating Response Surface Designs in Terms of The Mean Squared Error of Prediction", *Technometrics*, Vol. 33, 315-326.