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# 입방형 영역을 사용한 반응표면계획에서 블록효과를 평가하기 위한 측도

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# A Measure for Evaluating the Effect of Blocking in Response Surface Designs Using Cuboidal Regions

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## Abstract

The fitting of a response surface model and the subsequent exploration of the response surface are usually based on the assumption that the experimental runs are carried out under homogeneous conditions. This, however, may be quite often difficult to achieve in many experiments. To control such an extraneous source of variation, the response surface design should be arranged in several blocks within which homogeneity of conditions can be maintained. In this case, when fitting a response surface model, the least squares estimates of the model's parameters and the prediction variance will generally depend on how the response surface design is blocked. That is, 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. In this paper, we propose a measure for evaluating the effect of blocking of response surface designs using cuboidal regions.

# 1. Introduction

The conditions under which experimental trials are performed in a response surface design may not, in general, be homogeneous. In this case, blocking may be often carried out within-block homogeneity. In the statistical literature on response surface methodology, whenever a block design is used, the block effect is often considered to be fixed - that is, represented by a constant parameter in the assumed model. This effect can affect the estimation of the mean response and prediction variance over a certain region of interest. In particular, the least squares estimates of the coefficients associated with the input variables in the fitted model generally depend on the manner in which the design is divided into blocks. Furthermore, the design is frequently chosen so that it blocks orthogonally. In this special case, the least squares estimates and prediction variance are invariant to the block effect, and hence the standard techniques of response surface methodology can be applied as if the block effect did not exist. 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 $d(\geq 1)$.

In many experimental situations, a response surface design may not block orthogonally. 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 response when block effects are fixed.

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. The presence of a random block effect, in addition to the usual fixed 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 his work by the addition of interaction terms between the fixed polynomial effects and the random block effects.

Giovannitti-Jensen and Myers(1989) developed the notion of variance dispersion graphs(VDG) as a variance-based graphical technique for displaying a given standard design's performance for a specific model on spheres of varying radii inside a region of interest. 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. And Park and Jang(1997) proposed a measure and a graphical method for evaluating the effect of blocking in response surface designs with random block effects. This article extended the work of Park and Jang(1999a). Park and Jang(1999b) proposed another graphical method for evaluating the effect of blocking in response surface designs. All of the discussions and illustrations in the preceding papers deal 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.382).). Also, spheres nested inside the design cube can be used as the media for the VDG(See Myers et al.(1992).). However, 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 this paper, using the ideas proposed by Khuri(1992, 1994) and Rozum and Myers(1991), we propose a measure for evaluating the effect of blocking in response surface designs using cuboidal regions in terms of prediction variance. This measure can be used as a measure to investigate how blocking influences the prediction variance throughout the entire experimental region and to compare the effect of blocking in the cases of the orthogonal and non-orthogonal block designs, respectively.

## 2. Effect of Blocking on the Prediction Variance

### 2.1 Case of a fixed block effect

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

$$\eta(\underset{\sim}{x}) = \beta_0 + \underset{\sim}{x}_\beta{}' \underset{\sim}{\beta} \tag{1}$$

where the elements of the vector $\underset{\sim}{\beta} = (\beta_1, \beta_2, \cdots, \beta_p)'$ and $\beta_0$ are unknown constant parameters and $\underset{\sim}{x}_\beta{}'$ is a vector of order $1 \times p$ whose elements are model terms except the intercept. For a first-order model $\underline{x}_\beta' = (x_1, x_2, \cdots, x_k)$ and $\underline{\beta} = (\beta_1, \beta_2, \cdots, \beta_k)'$, and for a second-order model $\underline{x}_\beta' = (x_1, x_2, \cdots, x_k, x_1^2, x_2^2, \cdots, x_k, x_1^2, x_2^2, \cdots, x_k^2, x_1x_2, \cdots, x_1x_k, \cdots, x_{k-1}x_k)$ and $\underline{\beta} = (\beta_1, \beta_2, \cdots, \beta_k, \beta_{11}, \beta_{22}, \cdots, \beta_{kk}, \beta_{12}, \cdots, \beta_{1k}, \cdots, \beta_{(k-1)k})'$.

Let us assume that the experimental units used are not homogeneous, but that they can be divided into $b$ blocks, where the units within a block are somewhat homogeneous. Let $n_j$ denote the size of the $j$th 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

$$\underline{y} = \beta_0 \mathbf{1}_n + X\underline{\beta} + Z\underline{\delta} + \underline{\varepsilon} \qquad (2)$$

where $\mathbf{1}_n$ is a vector of ones of order $n \times 1$, $X$ is an $n \times p$ model matrix except $\mathbf{1}_n$, the elements of the vector $\underline{\beta} = (\beta_1, \beta_2, \cdots, \beta_p)'$ and $\beta_0$ are unknown constant parameters, $\underline{\delta} = (\delta_1, \delta_2, \cdots, \delta_b)'$ is a fixed factor, where $\delta_j$ denotes the effect of the $j$th block, $Z$ is a block-diagonal matrix of form $Z = diag(\mathbf{1}_{n_1}, \mathbf{1}_{n_2}, \cdots, \mathbf{1}_{n_b})$, and $\underline{\varepsilon}$ is an $n \times 1$ 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 $n \times n$. Since $\mathbf{1}_n = Z\mathbf{1}_b$, model (2) can be written as

$$\underline{y} = W\underline{\theta} + \underline{\varepsilon} \qquad (3)$$

where $W = [X : Z]$, $\underline{\theta} = (\underline{\beta}', \underline{\tau}')'$, and $\underline{\tau} = \beta_0 \mathbf{1}_b + \underline{\delta}$. If the block effects are constrained to sum to zero, that is, $\sum_{j=1}^{b} \delta_j = 0$, then $\beta_0$ can be expressed as

$$\beta_0 = \frac{1}{b} \sum_{j=1}^{b} \tau_j = \frac{1}{b} \mathbf{1}_b' \underline{\tau}$$

where $\tau_j$ is the $j$th element of $\underline{\tau}(j=1,2,\cdots,b)$. Then, the least-squares estimator of $\underline{\theta}$ is given by $\hat{\underline{\theta}} = (W'W)^{-1}W'\underline{y}$ and the variance-covariance matrix of $\hat{\underline{\theta}}$ is

$$Var(\hat{\underline{\theta}}) = (W'W)^{-1}\sigma_\varepsilon^2. \tag{4}$$

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

$$\hat{\eta}(\underline{x}) = \hat{\beta}_0 + \underline{x}_\beta'\hat{\underline{\beta}} \tag{5}$$

where $\hat{\beta}_0 = \frac{1}{b}\ \underline{1}_b'\hat{\underline{\tau}}$. Formula (5) can be rewritten as

$$\hat{\eta}(\underline{x}) = \underline{x}_\theta'\hat{\underline{\theta}} \tag{6}$$

where $\underline{x}_\theta' = [\ \underline{x}_\beta' : \frac{1}{b}\ \underline{1}_b']$. The prediction variance of $\hat{\eta}(\underline{x})$ can therefore be written as

$$Var[\ \hat{\eta}(\underline{x})] = \underline{x}_\theta'(W'W)^{-1}\underline{x}_\theta\sigma_\varepsilon^2. \tag{7}$$

Khuri(1994) demonstrated the following two results.

**Result 1.** Under orthogonal blocking, the prediction variance in formula (7) takes the form

$$Var[\ \hat{\eta}(\underline{x})] = Var[\ \hat{\eta}_0(\underline{x})] + \left[\frac{1}{b^2}\sum_{j=1}^{b}\frac{1}{n_j} - \frac{1}{n}\right]\sigma_\varepsilon^2 \tag{8}$$

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

$$Var[\ \hat{\eta}_0(\underline{x})] = \underline{x}_u'(U'U)^{-1}\underline{x}_u\sigma_\varepsilon^2 \tag{9}$$

where $\underline{x}_u' = [1 : \underline{x}_\beta']$ and $U = [\ \underline{1}_n : X]$.

**Result 2.** Under non-orthogonal blocking, the prediction variance in formula (7) takes the form

$$Var[\hat{\eta}(\underline{x})] = Var[\hat{\eta}_0(\underline{x})] + \underline{x}_\theta' Q \underline{x}_\theta \sigma_\varepsilon^2 \tag{10}$$

where $Q$ is the matrix of order $(p+b)\times(p+b)$ of the form $Q=(W'W)^{-1}M[M'(W'W)^{-1}M]^{-1}M'(W'W)^{-1}$, where $W=[X:Z]$, and $M'$ is a matrix of order $(b-1)\times(p+b)$ of the form $M'=[0:L]$, where $0$ is a zero matrix of order $(b-1)\times p$ and $L=[\underline{1}_{b-1}: -I_{b-1}]$ is of order $(b-1)\times b$.

From result 1, we can conclude that when the design blocks orthogonally, the prediction variance at a point $\underline{x}$ inside the experimental region exceeds $Var[\hat{\eta}_0(\underline{x})]$ by a constant amount that depends only on the sizes and number of the blocks. That is, since the second term on the right-hand side of formula (8) is nonnegative, we can find that blocking causes an increase in the prediction variance when the design blocks orthogonally. Result 2 implies that the amount of increase in the prediction variance, $\underline{x}_\theta' Q \underline{x}_\theta \sigma_\varepsilon^2$, is not necessarily constant at all points in the experimental region and that $Var[\hat{\eta}(\underline{x})] \geq Var[\hat{\eta}_0(\underline{x})]$ since $Q$ is positive semidefinite.

## 2.2 Case of a random block effect

Let us rewrite model (1) as

$$\eta(\underline{x}) = \underline{x}_u' \underline{\beta}^* \tag{11}$$

where $\underline{x}_u' = [1: \underline{x}_\beta']$ is denoted in formula (9) and $\underline{\beta}^* = [\beta_0 : \underline{\beta}']'$ is the vector of unknown constant parameters. Suppose that the experimental runs used to fit model (2) are not homogeneous due to the presence of an extraneous source of variation, denoted by $\underline{\delta}$, whose levels represent a random sample size $b$ from a much larger population. But they can be arranged in $b$ blocks, where the runs within a block are somewhat homogeneous. Let us represent model (2) as

$$\underline{y} = U\underline{\beta}^* + Z\underline{\delta} + \underline{\varepsilon} \tag{12}$$

where $U=[\underline{1}_n : X]$ denoted in formula (9) is an $n\times(p+1)$ model matrix and $\underline{\delta}$, $Z$ and $\underline{\varepsilon}$ are defined in model (2). This case deals with situations in which the block effect in model (12) is random so that $\underline{\delta}$ is distributed as $(\underline{0}, \sigma_\delta^2 I_b)$

independently of $\underline{\varepsilon}$. Model (12) is therefore a mixed model, since $\underline{\beta}^*$ is a fixed parameter vector. The mean response and the variance-covariance matrix of $\underline{y}$ are respectively $E(\underline{y}) = U\underline{\beta}^*$ and

$$\Sigma = \sigma_\varepsilon^2 I_n + \sigma_\delta^2 ZZ' = \sigma_\varepsilon^2 A \tag{13}$$

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

$$\zeta = \sigma_\delta^2 / \sigma_\varepsilon^2. \tag{14}$$

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

$$Var(\widehat{\underline{\beta}_g^*}) = (U'A^{-1}U)^{-1}\sigma_\varepsilon^2. \tag{15}$$

And the predicted value of the mean response in model (11) is given by

$$\widehat{\eta_g}(\underline{x}) = \underline{x}_u' \widehat{\underline{\beta}_g^*}. \tag{16}$$

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

$$Var[\widehat{\eta_g}(\underline{x})] = \underline{x}_u'(U'A^{-1}U)^{-1}\underline{x}_u\sigma_\varepsilon^2. \tag{17}$$

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 $\widehat{\underline{\beta}_o^*}$ of $\underline{\beta}^*$ obtained by ignoring the block effects is used as $\widehat{\underline{\beta}}_o^* = (U'U)^{-1}U'\underline{y}$ and the variance-covariance matrix of $\widehat{\underline{\beta}}_o^*$ is

$$Var(\widehat{\underline{\beta}}_o^*) = (U'U)^{-1}U'AU(U'U)^{-1}\sigma_\varepsilon^2. \tag{18}$$

And the predicted value of the mean response in model (11) is given by

$$\widehat{\eta}_o(\underline{x}) = \underline{x}_u{}'\widehat{\underline{\beta}}_o^*.$$

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

$$Var[\widehat{\eta}_o(\underline{x})] = \underline{x}_u{}'(U'U)^{-1}U'AU(U'U)^{-1}\underline{x}_u\sigma_\varepsilon^2. \tag{19}$$

Note that in a standard response surface model with no random effects, $\widehat{\underline{\beta}}_g^* = \widehat{\underline{\beta}}_o^* = \widehat{\underline{\beta}}^* = (U'U)^{-1}U'\underline{y}$, $Var(\widehat{\underline{\beta}}_g^*) = Var(\widehat{\underline{\beta}}_o^*) = Var(\widehat{\underline{\beta}}^*) = (U'U)^{-1}\sigma_\varepsilon^2$, and hence $Var[\widehat{\eta}_g(\underline{x})] = Var[\widehat{\eta}_o(\underline{x})] = Var[\hat{\eta}_0(\underline{x})]$.

## 3. A Measure for Evaluating the Effect of Blocking in Response Surface Designs Using Cuboidal Regions

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. These are all shown to be affected by the sizes of the blocks and the allocation of experimental runs to the blocks. Therefore, in order to examine the variation in the prediction variance after blocking, it would be important to choose a blocking arrangement in the same experimental designs. 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 in the presence of a fixed block effect. Using his idea, 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. Also, as the extension of their work, Park and Jang(1997) proposed a measure and a graphical method for evaluating the effect of blocking in response surface designs with random block effects.

All of the discussions and illustrations in the preceding papers deal with prediction variance for spherical regions of interest. In this case it is natural to observe values of $Var[\hat{\eta}(\underline{x})]/\sigma_\varepsilon^2$ 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. 382).). Also, spheres nested inside the design cube can be used as the media for the VDG(See Myers et al.(1992).). However, 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. Both are useful tools for comparing competing designs or blocking arrangements.

Thus, in order to investigate the variation in prediction variance caused by blocking, we introduce a measure that quantifies the effect of blocking in response surface designs using a cuboidal region in the cases of a fixed effect and a random effect, respectively.

## 3.1 Case of a fixed block effect

Since $\sigma_\varepsilon^2$ is generally unknown and beyond the control of the experimenter, it is important to note that, apart from the constant $\sigma_\varepsilon^2$, the prediction variance depends only on the design that determines the form of the assumed model and the specific location of $\underline{x}$. From formula (10), we define a measure as follows :

$$BEV_f(r) = K\int_C \underline{x}_\theta{}' Q\, \underline{x}_\theta d\underline{x} \tag{20}$$

which we call the blocking effect variance(BEV) in the presence of a fixed block effect. Here, the radius $r$ is defined as the distance from the center of the hypercube to its face, $C$ is the hypercube with a radius $r$ defined by $C=\{\underline{x}: -r \le x_i \le r,\ i=1,2,\cdots,k\}$ and $K^{-1}=\int_C d\underline{x}$ implies integration over the volume of the hypercube with a radius $r$. Hence, the blocking effect variance means the average of $\underline{x}_\theta{}' Q\, \underline{x}_\theta$ over the volume of the hypercube with a radius $r$. By applying a property of the trace, the blocking effect variance, $BEV_f(r)$, is written as

$$\begin{aligned} BEV_f(r) &= K\int_C tr[\ \underline{x}_\theta' Q\, \underline{x}_\theta]d\underline{x} \\ &= tr\left[K\int_C \underline{x}_\theta\ \underline{x}_\theta' Q d\underline{x}\right] \\ &= tr[SQ] \end{aligned} \tag{21}$$

where $S=K\int_C \underline{x}_\theta\ \underline{x}_\theta' d\underline{x}$ is a matrix of the cuboidal region moments.

A cuboidal region moment of order $q$ is defined as follows :

$$\sigma_{q_1 q_2 \cdots q_k} = K\int_C x_1^{q_1} x_2^{q_2} \cdots x_k^{q_k} d\underline{x} \tag{22}$$

where $K^{-1}=\int_C d\underline{x}=(2r)^k$ is the cuboidal volume of 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 $C$ is a symmetric region, the cuboidal region moment $\sigma_{q_1 q_2 \cdots q_k}$ is 0 whenever any $q_i$ is odd. The cuboidal region moments that are used in the development of the blocking effect variance for the first-order and second-order model cases are the second and fourth-order cuboidal region moments given by

$$\begin{aligned} \sigma_2 &= K\int_C x_i^2 d\underline{x} = \frac{r^2}{3}, \\ \sigma_4 &= K\int_C x_i^4 d\underline{x} = \frac{r^4}{5}, \\ \sigma_{22} &= K\int_C x_i^2 x_j^2 d\underline{x} = \frac{r^4}{9}. \end{aligned} \tag{23}$$

By applying formulas (22) and (23) to formula (21), we obtain, in the case of a first-order model,

$$BEV_f(r) = \frac{1}{b^2} \sum_{i=k+1}^{k+b} \sum_{j=k+1}^{k+b} c^{ij} + \frac{r^2}{3} \sum_{i=1}^{k} c^{ii}$$

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

$$BEV_f(r) = \frac{1}{b^2}\sum_{i=p+1}^{p+b}\sum_{j=p+1}^{p+b} c^{ij} + \frac{r^2}{3}\left(\sum_{i=1}^{k} c^{ii} + \frac{2}{b}\sum_{i=p+1}^{p+b}\sum_{j=k+1}^{2k} c^{ij}\right) + r^4\left\{\frac{1}{5}\sum_{i=k+1}^{2k} c^{ii} + \frac{1}{9}\left(\sum_{i=2k+1}^{p} c^{ii} + \sum_{i=k+1}^{2k}\sum_{\substack{j=k+1 \\ i\neq j}}^{2k} c^{ij}\right)\right\} \tag{24}$$

where $c^{ij}$ is the $(i,j)$th element of $Q$ $(i,j=1,2,\cdots,p+b)$. This quantity, $BEV_f(r)$, is the average of the amount of increase in the prediction variance over the volume of a cube with a radius $r$ due to blocking. Therefore, this quantity can be used as a measure for evaluating the effect of blocking on the prediction variance in response surface designs using cuboidal regions in the case of a fixed block effect. Also, this quantity can be used to measure the extent to which blocking in a given design is away from orthogonal blocking.

## 3.2 Case of a random block effect

From formulas (17) and (19), let us consider

$$V_B(\underline{x}) = \frac{Var[\widehat{\eta_g}(\underline{x})]}{\sigma_\varepsilon^2} = \underline{x}_u'(U'A^{-1}U)^{-1}\underline{x}_u \tag{25}$$

and

$$V_U(\underline{x}) = \frac{Var[\widehat{\eta_o}(\underline{x})]}{\sigma_\varepsilon^2} = \underline{x}_u'(U'U)^{-1}U'AU(U'U)^{-1}\underline{x}_u. \tag{26}$$

Thus, from formulas (25) and (26), we define measures as follows :

$$\begin{aligned} BEV_r^B(r) &= K\int_C V_B(\underline{x})d\underline{x} \\ &= K\int_C \underline{x}_u' Q_B\, \underline{x}_u d\underline{x} \end{aligned} \tag{27}$$

which we call the blocking effect variance in the presence of a random block effect and

$$\begin{aligned} BEV_r^U(r) &= K\int_C V_U(\underline{x})d\underline{x} \\ &= K\int_C \underline{x}_u' Q_U\, \underline{x}_u d\underline{x} \end{aligned} \tag{28}$$

which we call the unblocking effect variance in the presence of a random block effect. Here, $Q_B$ is the matrix of order $(p+1)\times(p+1)$ of the form $Q_B=(U'\Lambda^{-1}U)^{-1}$, $Q_U$ is the matrix of order $(p+1)\times(p+1)$ of the form $Q_U=(U'U)^{-1}U'\Lambda U(U'U)^{-1}$, $C$ and $K^{-1}$ are defined in formula (20). Similarly, by applying a property of the trace, formulas(27) and (28) are written as

$$\begin{aligned} BEV_r^B(r) &= K\int_C tr[\,\underline{x}_u{}'Q_B\,\underline{x}_u]d\underline{x} \\ &= tr\left[K\int_C \underline{x}_u\,\underline{x}_u{}'Q_B d\underline{x}\right] \\ &= tr[S^*Q_B] \end{aligned} \tag{29}$$

and

$$\begin{aligned} BEV_r^U(r) &= K\int_C tr[\,\underline{x}_u{}'Q_U\,\underline{x}_u]d\underline{x} \\ &= tr\left[K\int_C \underline{x}_u\,\underline{x}_u{}'Q_U d\underline{x}\right] \\ &= tr[S^*Q_U] \end{aligned} \tag{30}$$

where $S^*=K\int_C \underline{x}_u\,\underline{x}_u{}'d\underline{x}$ is a matrix of the cuboidal region moments. Using the cuboidal region moments in formulas (22) and (23) for reexpression of formulas (29) and (30), we obtain, in the case of a first-order model,

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

and

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

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

$$\begin{aligned} BEV_r^B(r)= \; & d^{00}+\frac{r^2}{3}\left(\sum_{i=1}^{k}d^{ii}+2\sum_{i=k+1}^{2k}d^{1i}\right) \\ & +r^4\left\{\frac{1}{5}\sum_{i=k+1}^{2k}d^{ii}+\frac{1}{9}\left(\sum_{i=2k+1}^{p}d^{ii}+\sum_{i=k+1}^{2k}\sum_{\substack{j=k+1\\ i\neq j}}^{2k}d^{ij}\right)\right\} \end{aligned} \tag{31}$$

and

$$BEV_r^U(r) = e^{00} + \frac{r^2}{3}\left(\sum_{i=1}^{k} e^{ii} + 2\sum_{i=k+1}^{2k} e^{1i}\right) + r^4\left\{\frac{1}{5}\sum_{i=k+1}^{2k} e^{ii} + \frac{1}{9}\left(\sum_{i=2k+1}^{p} e^{ii} + \sum_{i=k+1}^{2k}\sum_{\substack{j=k+1\\ i\neq j}}^{2k} e^{ij}\right)\right\} \tag{32}$$

where $d^{ij}$ is the $(i,j)$th element of $Q_B(i,j=0,1,2,\cdots,p)$ and $e^{ij}$ is the $(i,j)$th element of $Q_U(i,j=0,1,2,\cdots,p)$. The quantity, $BEV_r^B(r)$, is the average of the prediction variances over the volume of a hypercube with a radius $r$ due to blocking when there are block effects and the quantity, $BEV_r^U(r)$, is the average of the prediction variances obtained by ignoring the block effects over the volume of a hypercube with a radius $r$ when there are block effects. Hence, $BEV_r^B(r)$ and $BEV_r^U(r)$ can be used as a measure for evaluating the effect of blocking on the prediction variance in response surface designs using cuboidal regions in the case of a random block effect.

Thus, through these measures, $BEV_f(r)$, $BEV_r^B(r)$ and $BEV_r^U(r)$, we can examine more clearly the variation in the prediction variance resulting from blocking in the cases of a fixed and random effect, throughout the entire experimental regions of interest, when these regions are cuboidal, and compare the block effects in the cases of the orthogonal and non-orthogonal block designs, respectively. Therefore, given the same number of experimental runs, we can choose between competing blocking arrangements one which is more effective in terms of prediction variance when the region of interest is cuboidal.

## 4. A Numerical Example

Let us consider the example used in Khuri(1994). 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 I> shows the original block 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 original block 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. Let us consider other blocking arrangements of the same 24 experimental runs in <Table I>. These blocking arrangements are described in <Table II>, which is modified from <Table II> in Khuri(1994). All blocking arrangements are scaled so that the design perimeter is restricted to being inside a unit cube. For each blocking arrangement, computations of the blocking effect variances are made. The results are given in <Table III>. It should be noted that the original and blocking arrangement 6 is orthogonal, but the other blocking arrangements are not. It also should be noted that blocking arrangements 1~5 except blocking arrangement 6 have the same number of blocks and block sizes as in the original block design, but the allocation of experimental runs to the blocks is not the same.

< Table I > The original block design

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

< Table II > Division of the experimental runs described in Table I for the blocking arrangements

| Blocking arrangement | Block 1 | Block 2 | Block 3 | Block 4 |
|---|---|---|---|---|
| 1 | 1, 2, 5<br>6, 11, 12 | 3, 4, 7<br>8, 9, 10 | 13, 14, 15<br>16, 17, 18 | 19, 20, 21<br>22, 23, 24 |
| 2 | 3, 4, 5<br>6, 13, 14 | 9, 10, 11<br>12, 19, 20 | 1, 2, 15<br>16, 17, 18 | 7, 8, 21<br>22, 23, 24 |
| 3 | 2, 3, 4<br>5, 6, 13 | 8, 9, 10<br>11, 12, 19 | 1, 14, 15<br>16, 17, 18 | 7, 20, 21<br>22, 23, 24 |
| 4 | 1, 2, 3<br>4, 5, 13 | 7, 8, 9<br>10, 11, 19 | 6, 14, 15<br>16, 17, 18 | 12, 20, 21<br>22, 23, 24 |
| 5 | 3, 4, 5<br>6, 13, 14 | 7, 8, 9<br>10, 11, 12 | 1, 2, 15<br>16, 17, 18 | 19, 20, 21<br>22, 23, 24 |
| 6 | 1, 2, 3, 4<br>5, 6, 7, 8<br>9, 10, 11, 12 | 13, 14, 15<br>16, 17, 18 | 19, 20, 21<br>22, 23, 24 | |

< Table III > The blocking effect variances for blocking arrangements with a fixed effect

| | Blocking arrangement | | | | | | |
|---|---|---|---|---|---|---|---|
| | original* | 1 | 2 | 3 | 4 | 5 | 6* |
| BEV | 0.0000 | 0.1398 | 0.1061 | 0.0281 | 0.0157 | 0.0426 | 0.0046 |

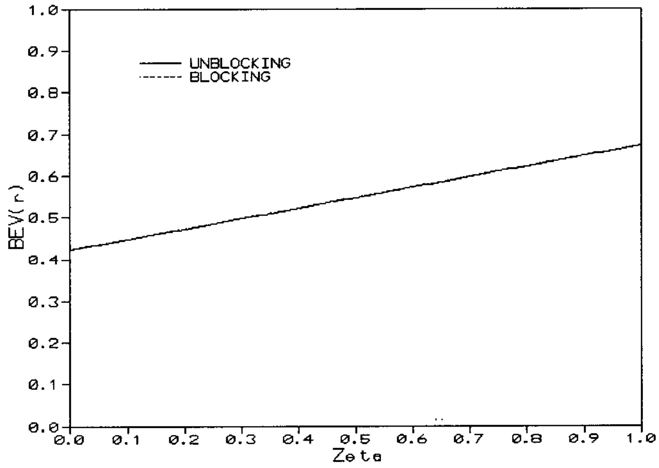
* Orthogonal blocking arrangements

### 4.1 Case of a fixed block effect

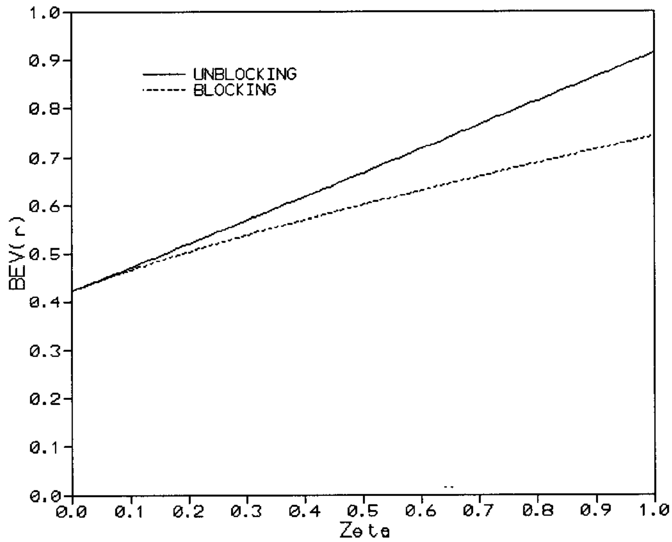
From <Table III>, we can find that since the original design blocks orthogonally and has the same block sizes, we can find that the values of the BEV in equation (24) are equal to zero. Hence, for this blocking arrangement, blocking causes no increase in the prediction variance. But, we see that since blocking arrangement 6 is an orthogonal blocked design which has the different block sizes, the value of BEV is not zero. Also, in the cases of the non-orthogonal blocking arrangements 1~5 which have the same number of blocks and block sizes, we can clearly see that blocking arrangement 4 minimizes the average increase in the prediction variance caused by blocking. These results are the same as those of Park and Jang(1999a) obtained in terms of spherical regions.

### 4.2 Case of a random block effect

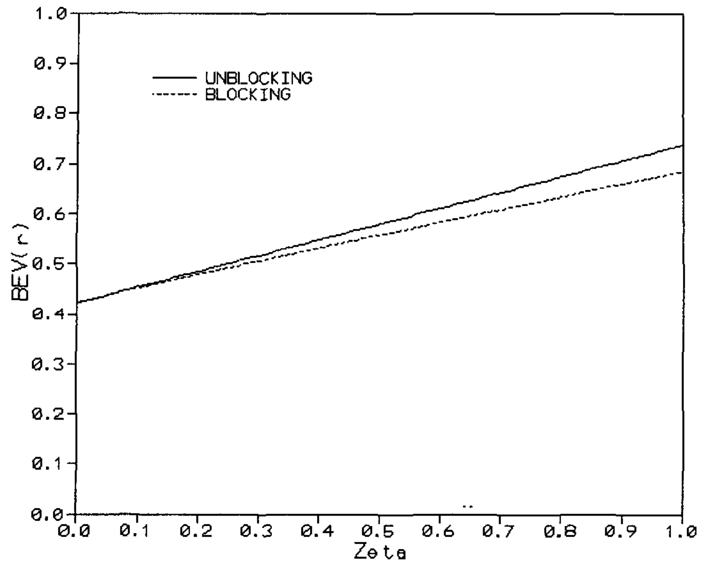
We shall consider the same example and blocking arrangements used in the previous case of a fixed block effect. In this case of a random block effect, it must be considered the value of the ratio $\zeta = \sigma_\delta^2 / \sigma_\varepsilon^2$. In general, the ratio $\zeta$ is unknown and should therefore be estimated from the data. However, since our concerns is merely in the performance of an experimental design, according to the various values of $\zeta$ with an appropriate size ($\zeta = 0 \sim 1.0$), computations of the blocking effect variances and the unblocking effect variances for several blocking arrangement in Table II are made, respectively. As the results, we have tried to depict the graphs of the blocking effect variances and the unblocking effect variances for several blocking arrangements against varying $\zeta$. From these Figures, we find that on the whole, the unblocking effect variances and the blocking effect variances of the blocking arrangements increase as $\zeta$ increases and the unblocking effect variances for the blocking arrangements are always greater than or equal to the blocking effect variances. That is, $Var[.\ \widehat{\eta}_o(\underset{\sim}{x})] \geq Var[\ \widehat{\eta}_g(\underset{\sim}{x})]$ against varying $\zeta$ in the presence of a random block effect. <Figure 1> and 4 show the graphs of the blocking effect variances and the unblocking effect variances for orthogonal blocked designs with a random effect against varying $\zeta$. From <Figure 1>, we can find that since the original design blocks orthogonally and has the same block sizes, the unblocking effect variances and the blocking effect variances are same for against varying $\zeta$. But from <Figure 4>, because blocking arrangement 6 has the different block sizes, though the design blocks orthogonally, the unblocking effect variances and the blocking effect variances always are not same for against varying $\zeta$. <Figure 2> and 3 show the graphs of blocking arrangements such that the average change in the prediction variance due to blocking is very high and low respectively, among the non-orthogonal blocking arrangements $1 \sim 5$ which have the same number of blocks and block sizes. Comparing the non-orthogonal blocking arrangements $1 \sim 5$, from <Figure 3>, we can see that for any values of $\zeta$, blocking arrangement 4 among blocking arrangements $1 \sim 5$ is most effective in terms of prediction variance. <Figure 5> shows differences between the unblocking effect variances and the blocking effect variances for several blocking arrangements with a random effect against various $\zeta$. From <Figure 5>, we can see more clearly the change of the block effects for several blocking arrangements. <Figure 6> shows comparison of the blocking effect variances for several blocking arrangements with a random effect against various $\zeta$. From <Figure 6>, we can see that for any values of $\zeta$, the original block design is most effective among several blocking arrangements. These results are the same results as those of Park and Jang(1997) obtained in terms of spherical regions.



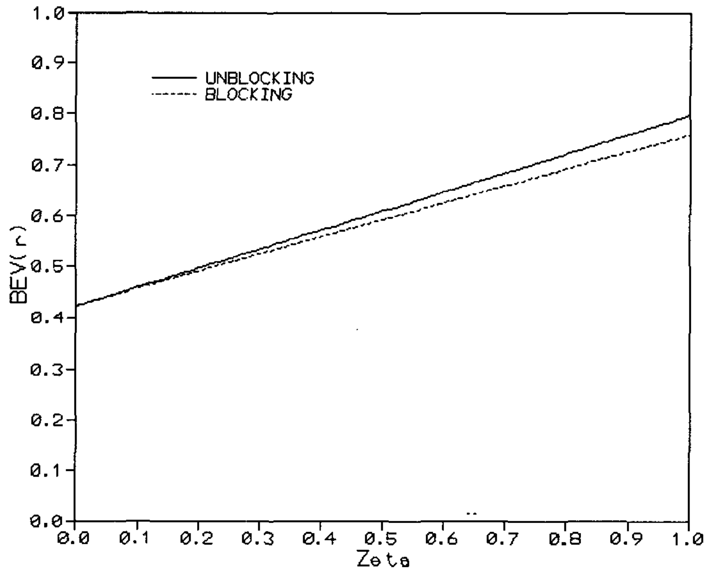

< Figure 1 > Blocking effect variances for the original block design with a random effect against varying $\zeta$



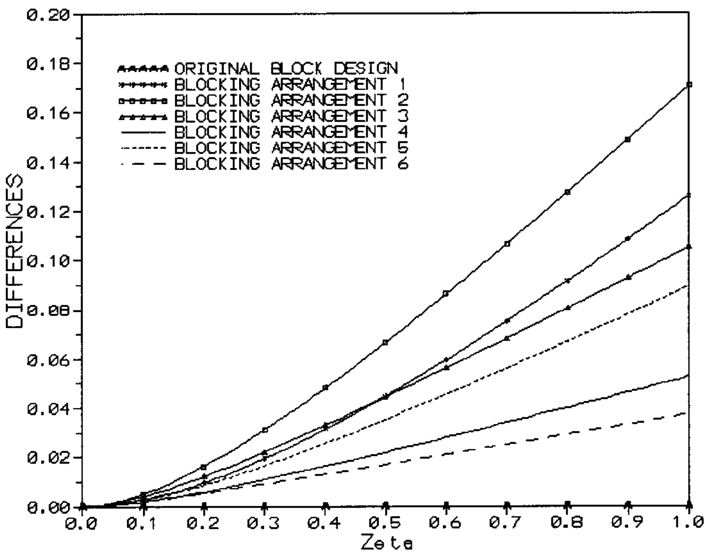

< Figure 2 > Blocking effect variances for blocking arrangement 2 with a random effect against varying $\zeta$



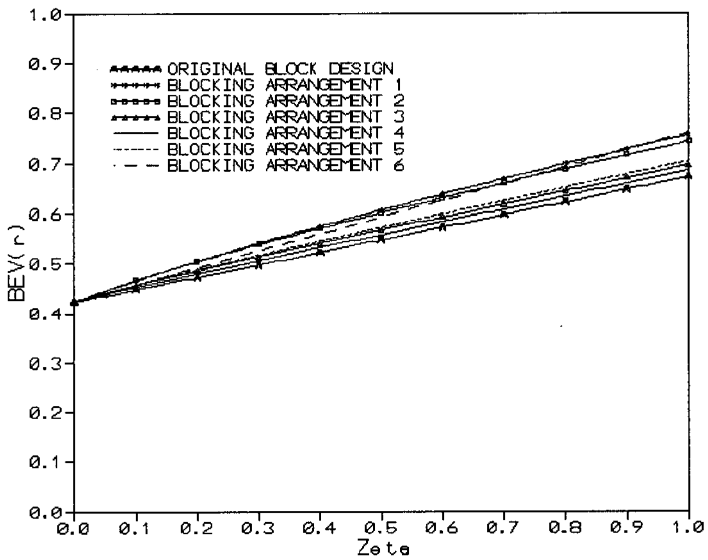

< Figure 3 > Blocking effect variances for blocking arrangement 4 with a random effect against varying $\zeta$




< Figure 4 > Blocking effect variances for blocking arrangement 6 with a random effect against varying $\zeta$




< Figure 5 > Differences between the unblocking effect variances and the blocking effect variances for several blocking arrangements with a random effect against varying $\zeta$




< Figure 6 > Blocking effect variances for several blocking arrangements with a random effect against varying $\zeta$

# 5. Conclusions

In many RSM situations the study is too large to allow all runs to be made under homogeneous conditions. As a result, it is important and interesting to consider the experimental designs that facilitate blocking, that is, the inclusion of block effects. Also, 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. Therefore, care should be exercised in the selection of blocks.

In this paper, a measure, the BEV has been proposed that allows us to evaluate the block effects in response surface designs using cuboidal regions. Computing the blocking effect variances and the unblocking effect variances in the presence of a fixed and random effect, we can evaluate and compare the effect of blocking on the prediction variance in the cases of the orthogonal and non-orthogonal blocked designs, respectively, when the region of interest is cuboidal. In the case of a fixed effect, the average increase in prediction variance of any blocked design resulting from blocking appears to be always greater than or equal to zero. But in the case of a random effect, the average of the prediction variances of an unblocked design obtained by ignoring the block effects appears to be always higher than that of the corresponding blocked design. Therefore, through this measure, we ascertain that which block design minimizes the average change in the prediction variance caused by blocking, and this measure allows us to compare and evaluate any blocked designs with a fixed and random effect in terms of prediction variance when the region of interest is cuboidal.

Considering 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.

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