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A Graphical Method for Evaluating the Effect of Blocking in Response Surface Designs Using Cuboidal Regions

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Abstract

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 even if the experimental runs are the same. Therefore, care should be exercised in the selection of blocks. In this paper, we propose a graphical method for evaluating the effect of blocking in a response surface designs using cuboidal regions in the presence of a fixed block effect. This graphical method can be used to investigate how the blocking has influence on the prediction variance throughout the entire experimental region of interest when this region is cuboidal, and compare the block effect in the cases of the orthogonal and non-orthogonal block designs, respectively.

1. Introduction

Model fitting in response surface methodology is 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 blocks within which homogeneity of conditions can be maintained. This block effect can affect the estimation of the mean response and its prediction variance over a certain region of interest. In particular, the least squares estimates of the coefficients and prediction variance 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

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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. In all such cases, the least squares fit of the assumed model and prediction variance can be affected by the blocking arrangement even if the experimental runs are the same. 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 in the presence of a fixed block effect.

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. Using the concepts of Khuri(1994) and Giovannitti-Jensen and Myers(1989), in the presence of a fixed block effect, Park and Jang(1997a) proposed measures for evaluating the effect of blocking in response surface designs in terms of prediction variance. And using the ideas proposed by Khuri(1992, 1994) and Giovannitti-Jensen and Myers(1989), Park and Jang(1997b) 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 works of Park and Jang(1997a).

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(1992, 1994) and Rozum and Myers(1991), Park and Jang(1998) proposed a measure for evaluating the effect of blocking in response surface designs using cuboidal regions.

In this paper, using the ideas proposed by Khuri(1992, 1994), 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 using cuboidal regions in the presence of a fixed block effect. This graphical method can be used to assess graphically the overall increase in the prediction variance resulting from blocking, throughout the entire experimental regions of interest, when this region is cuboidal, and compare the block effect in the cases of the orthogonal and non-orthogonal block designs, respectively. The drawback of the numeric measures proposed by Park and Jang(1997a) and Park and Jang(1998) 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.

2. Effect of Blocking on the Prediction Variance

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, $\eta(\underline{x})$, at a point $\underline{x} = (x_1, x_2, \cdots, x_k)'$ inside a region of interest R is given by

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

where the elements of the vector $\underline{\beta} = (\beta_1, \beta_2, \cdots, \beta_p)'$ and β_0 are unknown constant parameters, $\underline{x}_\beta{}'$ is a vector of order $1 \times p$ whose elements consist of the x_i terms along with their powers and cross-products of these powers up to a degree d. 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 $\underline{x}_\beta{}' = (x_1, x_2, \cdots, x_k, x_1^2, x_2^2, \cdots, x_k^2, x_1x_2, \cdots, x_1x_k, \cdots, x_{k-1}x_k)$ and $\underline{\beta} = (\beta_1, \beta_2, \cdots, \beta_k, \beta_{11}, \beta_{22}, \cdots, \beta_{kk}, \beta_{12}, \cdots, \beta_{1k}, \cdots, \beta_{k-1k})'$.

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 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

$$\underline{y} = \beta_0 \underline{1}_n + X\underline{\beta} + Z\underline{\delta} + \underline{\varepsilon} \tag{2}$$

where $\underline{1}_n$ is a vector of ones of order $n \times 1$, X is an $n \times p$ model matrix except $\underline{1}_n$, the elements of the vector $\underline{\beta} = (\beta_1, \beta_2, \cdots, \beta_p)'$ and β_0 are unknown constant parameters, $\underline{\delta} = (\delta_1, \delta_2, \cdots, \delta_b)'$, where δ_j denotes the effect of the jth block, Z is a block-diagonal matrix of form $Z = diag(\underline{1}_{n_1}, \underline{1}_{n_2}, \cdots, \underline{1}_{n_b})$, 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 $n \times n$. Since $\underline{1}_n = Z\underline{1}_b$, model (2) can be written as

$$\underline{y} = W\underline{\theta} + \underline{\varepsilon} \tag{3}$$

where $W = [X : Z]$, $\underline{\theta} = (\underline{\beta}', \underline{\tau}')'$, and $\underline{\tau} = \beta_0 \underline{1}_b + \underline{\delta}$. If the block effects are constrained to sum to zero, that is, $\sum_{j=1}^{b}\delta_j=0$, then β_0 can be expressed as

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

where τ_j is the jth 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 response 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 of the block. 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. From result 2, we can investigate that unlike the case of orthogonal blocking, the increase in the prediction variance, $\underline{x}_\theta' Q \underline{x}_\theta \sigma_\varepsilon^2$, is not necessarily constant at all points of the experimental region, and that because Q is positive semidefinite, $\underline{x}_\theta' Q \underline{x}_\theta \geq 0$ for all $\underline{x}$ and $Var[\hat{\eta}(\underline{x})] \geq Var[\hat{\eta}_0(\underline{x})]$.

3. A Graphical Method 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. In particular, in the case of a fixed block effect, it has been proved that the prediction variance increases as a result of blocking as shown in the previous results. Therefore, so as to investigate the overall increase in the prediction variance due to blocking, it would be important to choose a blocking arrangement in the same experimental runs.

In order to investigate the overall increase in the prediction variance resulting from blocking, we introduce a graphical method that quantifies the effect of blocking in response surface designs using cuboidal regions in the presence of a fixed block effect. Since σ_ε^2 is generally unknown and beyond the control of the experimenter, it is important to note that, with the exception of the constant σ_ε^2, the prediction variance depends only on the design and the form of the assumed model and the specific location of $\underline{x}$.

Thus, from formula (10), we define a quantity given by

$$V_{avg}(r) = \psi \int_{C_r} \underline{x}_\theta' Q \underline{x}_\theta d\underline{x} \tag{11}$$

which is called as the cuboidal increasing variance 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_r is the surface of a hypercube with a radius r defined by $C_r = \{\underline{x} : x_j = \pm r, -r \leq x_i \leq r, i \neq j, j = 1, 2, \cdots, k\}$ and $\psi^{-1} = \int_{C_r} d\underline{x}$ implies integration over the surface of the hypercube with a radius r. Hence, the cuboidal increasing variance means the average of $\underline{x}_\theta' Q \underline{x}_\theta$ over the surface of a hypercube with a radius r. By applying a property of a trace, $V_{avg}(r)$ is written as

$$\begin{aligned} V_{avg}(r) &= \psi \int_{C_r} tr[\underline{x}_\theta' Q \underline{x}_\theta] d\underline{x} \\ &= tr\left[\psi \int_{C_r} \underline{x}_\theta \underline{x}_\theta' Q d\underline{x}\right] \\ &= tr[CQ] \end{aligned} \tag{12}$$

where $C=\psi\int_{C_r} \underline{x}_\theta\ \underline{x}_\theta' d\underline{x}$ 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 $C_r=\{\underline{x}:x_j=\pm r, -r\le x_i\le r, i\ne j, j=1,2,\cdots,k\}$. Let

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

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 ;

$$\begin{aligned}\sigma_{q_1q_2\cdots q_k}&=\psi\int_{C_r} x_1^{q_1}x_2^{q_2}\cdots x_k^{q_k} d\underline{x}\\ &=2\psi\sum_{j=1}^{k}\int_{-r}^{r}\cdots\int_{-r}^{r} x_1^{q_1}x_2^{q_2}\cdots x_k^{q_k} dx_1\cdots dx_{j-1}dx_{j+1}\cdots dx_k\end{aligned} \tag{13}$$

where $\psi^{-1}=\int_{C_r} d\underline{x}=k2^k r^{k-1}$ 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 measure for the first-order and second-order model cases are the second and fourth order cuboidal region moments given by

$$\begin{aligned}\sigma_2&=\psi\int_{C_r} x_i^2 d\underline{x}=\frac{(k+2)r^2}{3k},\\ \sigma_4&=\psi\int_{C_r} x_i^4 d\underline{x}=\frac{(k+4)r^4}{5k},\\ \sigma_{22}&=\psi\int_{C_r} x_i^2x_j^2 d\underline{x}=\frac{(k+4)r^4}{9k}.\end{aligned} \tag{14}$$

By applying formulas (13) and (14) to formula (12), we obtain that in the case of a first-order model,

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

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

$$\begin{aligned}V_{avg}(r)=&\frac{1}{b^2}\sum_{i=p+1}^{p+b}\sum_{j=p+1}^{p+b} c^{ij}+\frac{(k+2)r^2}{3k}\left(\sum_{i=1}^{k} c^{ii}+\frac{2}{b}\sum_{i=p+1}^{p+b}\sum_{j=k+1}^{2k} c^{ij}\right)\\ &+\frac{(k+4)r^4}{k}\left\{\frac{1}{5}\sum_{i=k+1}^{2k} c^{ii}+\frac{1}{9}\left(\sum_{i=2k+1}^{p} c^{ii}+\sum_{i=k+1}^{2k}\sum_{\substack{j=k+1\\ i\ne j}}^{2k} c^{ij}\right)\right\}\end{aligned} \tag{15}$$

where c^{ij} is the (i,j)th element of Q $(i,j=1,2,\cdots,p+b)$. This quantity, $V_{avg}(r)$, is the average of increasing amount in the prediction variance resulting from blocking over the surface of a hypercube with a radius r in the case of a fixed block effect.

Also, from formula (10), let us consider

$$V_{\max}(r) = \max_{x \in C_r} [\ \underset{\sim}{x}_\theta{}' Q \underset{\sim}{x}_\theta] \tag{16}$$

and

$$V_{\min}(r) = \min_{x \in C_r} [\ \underset{\sim}{x}_\theta{}' Q \underset{\sim}{x}_\theta] \tag{17}$$

where $C_r = \{\underset{\sim}{x} : x_j = \pm r, -r \le x_i \le r,\ i \ne j, j = 1, 2, \cdots, k\}$. Then, it is required that the quantities, $V_{\max}(r)$ and $V_{\min}(r)$, be maximized and minimized over locations on a hypercube. These quantities, $V_{\max}(r)$, $V_{avg}(r)$ and $V_{\min}(r)$ can be used as a graphical measure to assess graphically the overall increase 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, $V_{\max}(r)$, $V_{avg}(r)$ and $V_{\min}(r)$, against the radius r. We call this graph the blocking effect graph(BEG) in the case of a fixed block effect when this region is cuboidal.

Through these graphs, we can examine more clearly the overall increase of the prediction variances after blocking against a radius r and compare the block effects in the cases of the orthogonal and non-orthogonal block designs, respectively. Hence, in the presence of a fixed block effect, we can clearly see that the which blocking arrangement in the same experimental design is most effective in terms of prediction variance when this region 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). A second order model in x_1, x_2 and x_3 was fitted using the design given Table 1. 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). All blocking arrangements are scaled so that the design perimeter is restricted to being inside a unit cube. For the basic design and several blocking arrangements described in Table 2, computations are made of the maximum, the average and the minimum of the increasing prediction variances, that is, $V_{\max}(r)$, $V_{avg}(r)$ and $V_{\min}(r)$. It should be noted that blocking

Table 1. The basic 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	$\sqrt{2}$

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 ~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 ~6 show blocking effect graph for several blocking arrangements with a fixed effect against a radius r in a cuboidal region. The BEGs show the dispersion in the increasing prediction variances as the radius r increases. From these Figures, we can clearly see the change of the block effects for each blocking arrangement as a radius r varies. From Figure 1, we can find that since the basic design blocks orthogonally and has the same block sizes, the BEG for the basic design appears in a straight line which has the same values against a radius r - all the values of $V_{\max}(r)$, $V_{avg}(r)$ and $V_{\min}(r)$ are zero against a radius r. This means that for this blocking arrangement, blocking causes no increase in the prediction variance. And from this Figure 1, we can find that because blocking arrangement 6 is also orthogonal, the BEG for this blocking arrangement 6 appears in a straight line which has the same values against a radius r, but all the values of $V_{max}(r)$, $V_{avg}(r)$ and $V_{min}(r)$ are not zero against a radius r because of the different block sizes. Also, we can find the fact that all the values of $V_{max}(r)$, $V_{avg}(r)$ and $V_{min}(r)$ for all blocking arrangements are always greater than or equal to 0.

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

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

Comparing the non-orthogonal blocking arrangements 1 ~5 which have the same number of blocks and the same block sizes, we can see that the dispersions for each blocking arrangements become wider gradually as a radius r increases and the dispersion of blocking arrangement 3 or 4 appears to be lowest. In particular, the BEG for blocking arrangements 1 shows that the maximum of the increasing prediction variance increases dramatically beyond a radius of about 0.63.

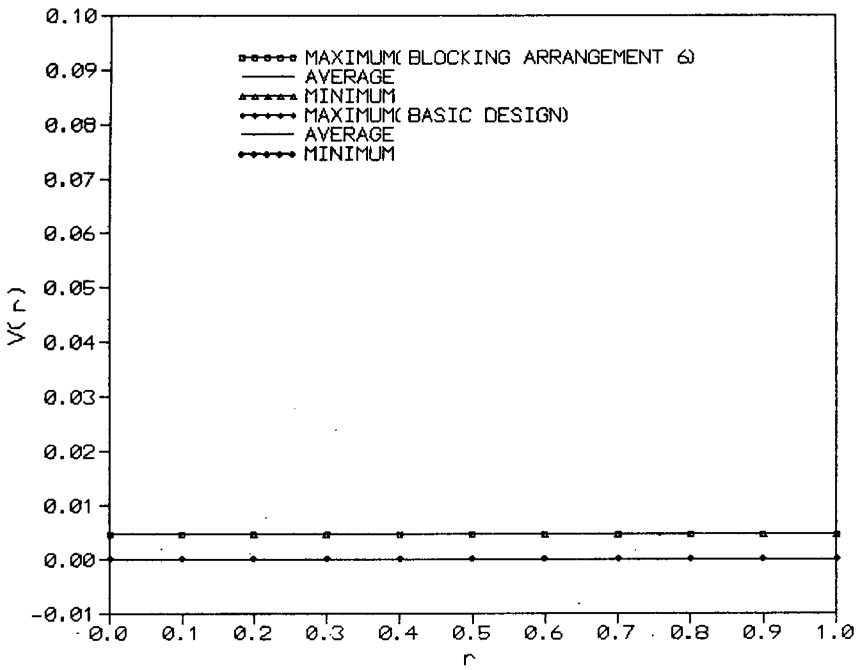

Figure 1. Blocking effect graph for the basic design and blocking arrangement 6 with a fixed effect against the radius r in a cuboidal region

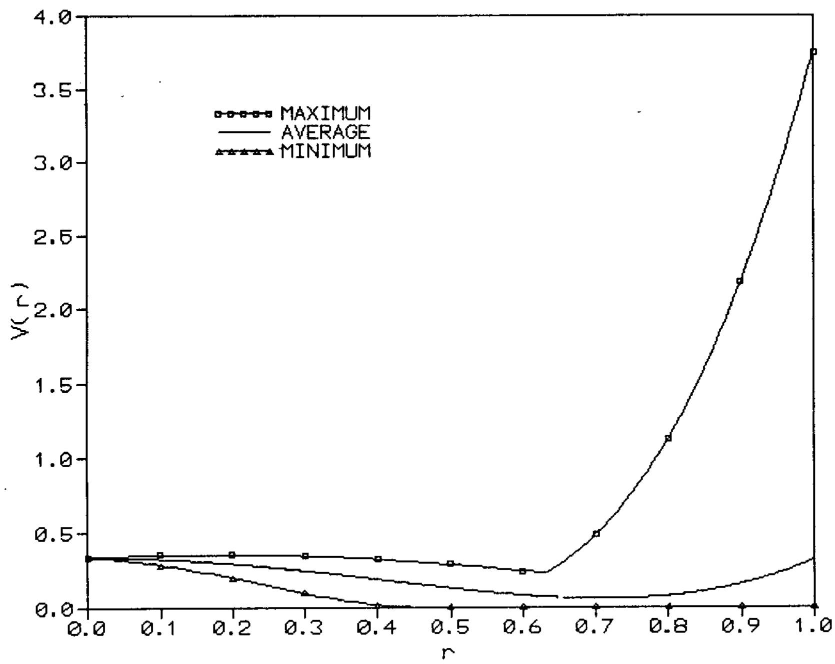

Figure 2. Blocking effect graph for blocking arrangement 1 with a fixed effect against the radius r in a cuboidal region

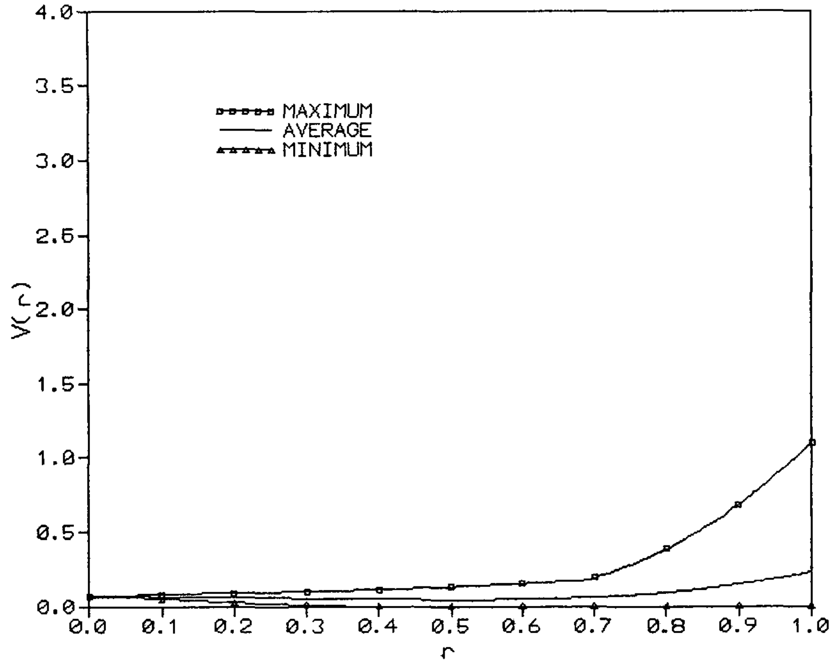

Figure 3. Blocking effect graph for blocking arrangement 2 with a fixed effect against the radius r in a cuboidal region

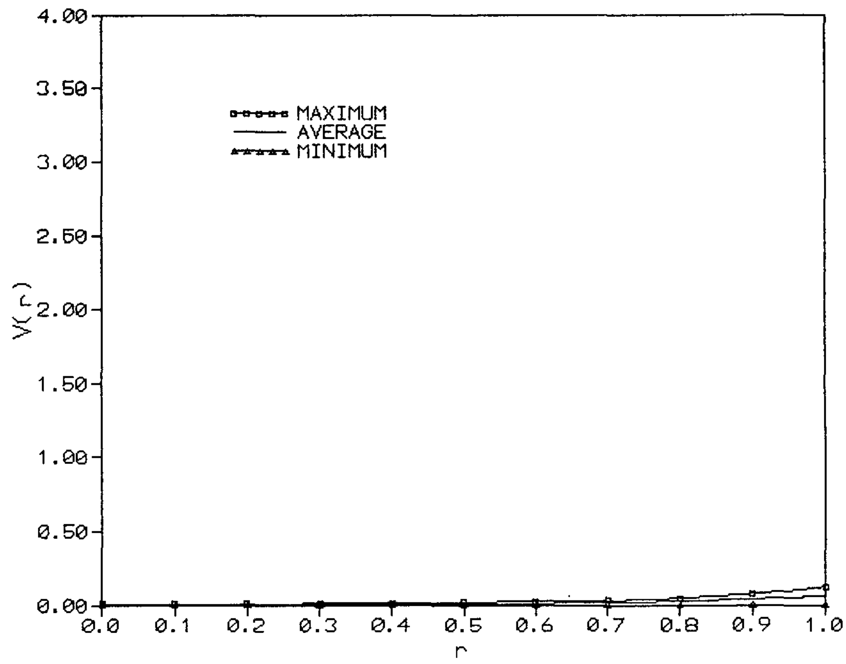

Figure 4. Blocking effect graph for blocking arrangement 3 with a fixed effect against the radius r in a cuboidal region

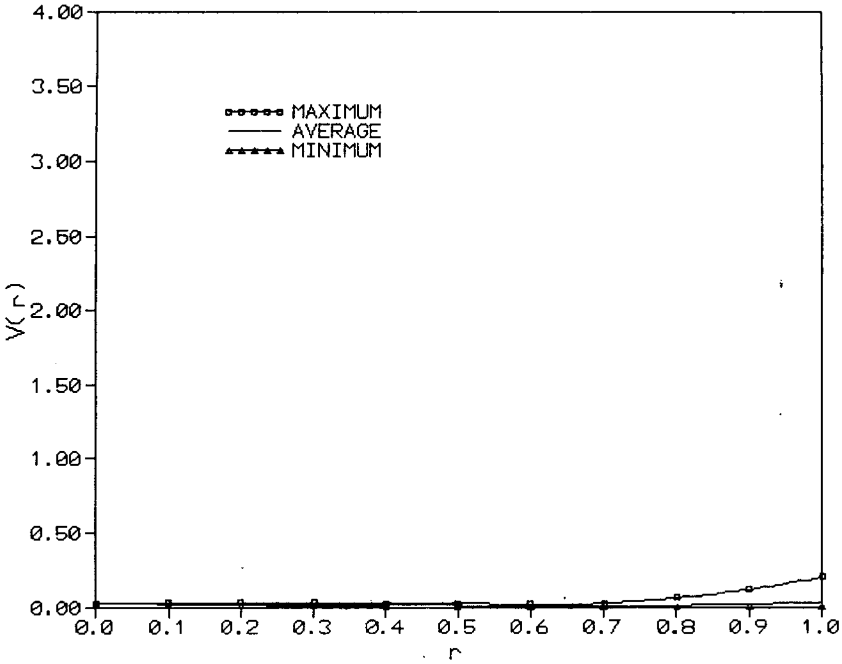

Figure 5. Blocking effect graph for blocking arrangement 4 with a fixed effect against the radius r in a cuboidal region

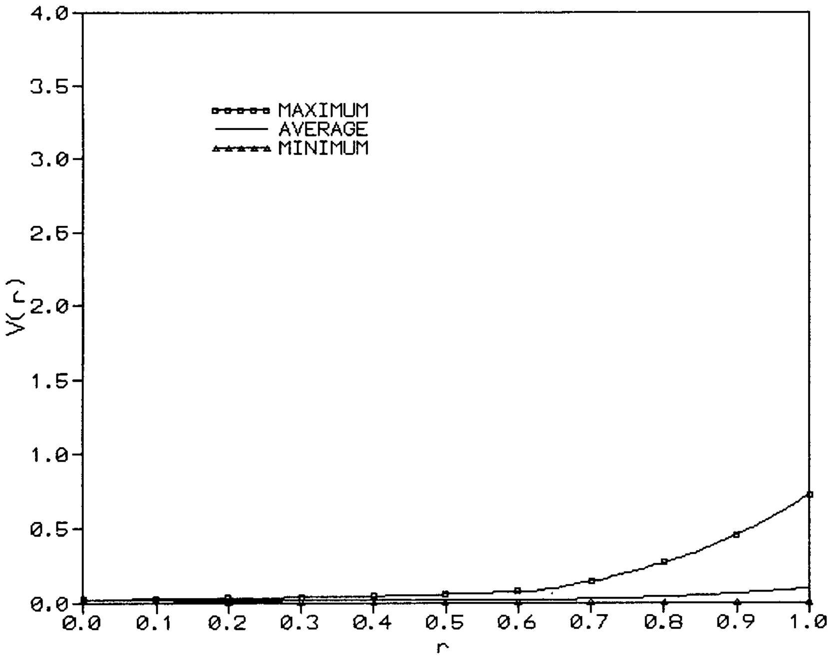

Figure 6. Blocking effect graph for blocking arrangement 5 with a fixed effect against the radius r in a cuboidal region

Figure 7 shows the cuboidal increasing variances for several blocking arrangements with a fixed effect against the radius r in a cuboidal region and Figure 8 shows the cuboidal increasing variances for several non-orthogonal blocking arrangements with a fixed effect against the radius r in a cuboidal region. In Figure 7 and Figure 8, the BEGs compare only the average of the increasing prediction variance for each blocking arrangement. From these Figures, we can obtain the same results as those obtained from the previous BEGs. From Figure 8, comparing the non-orthogonal blocking arrangements 1 ~5 which have the same number of blocks and block sizes, we can see that if the radius r is less than approximately 0.57, blocking arrangement 3 minimizes the overall increase in the prediction variance and blocking arrangement 4 minimizes beyond a radius of approximately 0.57. That is, we can find the fact that if the radius r is less than approximately 0.57, blocking arrangement 3 among the non-orthogonal blocking arrangements is most effective and blocking arrangement 4 is most effective beyond a radius of approximately 0.57 in terms of the prediction variance. In particular, from this figure, we can find that as the radius r increases, the cuboidal increasing variance of blocking arrangement 1 appears to be highest at the center of the design region and decreases gradually, and then the cuboidal increasing variance increases again near the perimeter of the design region. These results are similar to those of Park and Jang(1997a) obtained in terms of spherical regions.

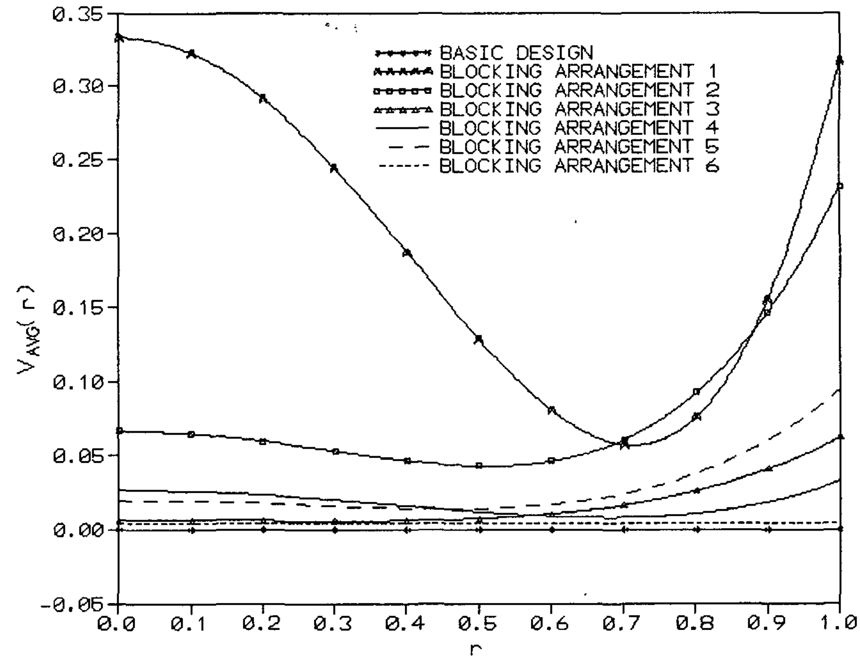

Figure 7. The cuboidal increasing variances for several blocking arrangements with a fixed effect against the radius r in a cuboidal region

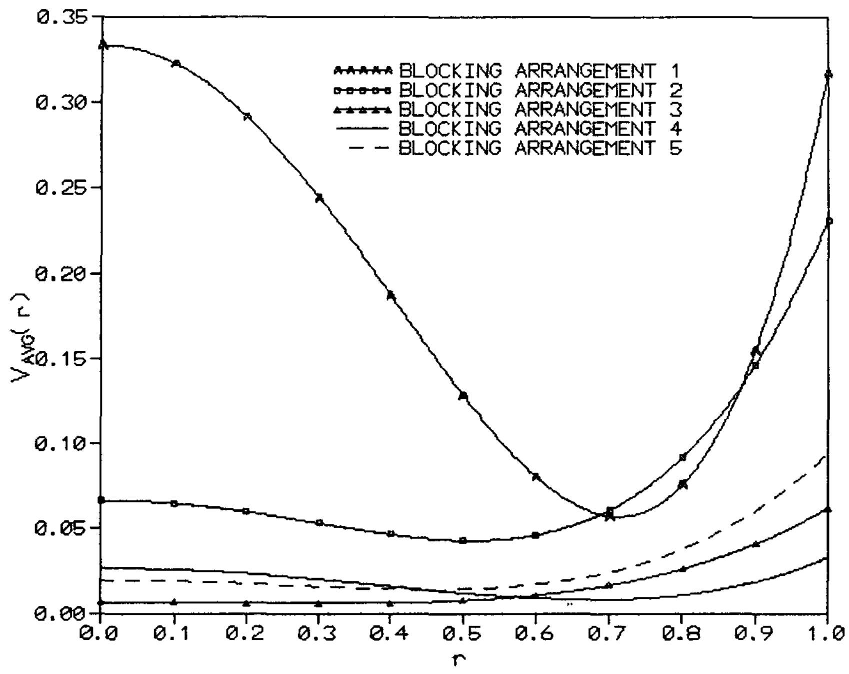

Figure 8. The cuboidal increasing variances for several non-orthogonal blocking arrangements with a fixed effect against the radius r in a cuboidal region

5. Conclusions

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. Blocking can increase the prediction variance. Therefore, care should be exercised in the selection of blocks. Unfortunately, single-valued criteria often fail to convey the true picture of a design's support for the fitted model, but the proposed graphical method describes what happens inside a region of interest, and provides better comparisons among blocking arrangements.

In this paper, a graphical method has been proposed that allows us to evaluate the effect of blocking in response surface designs using cuboidal regions in the case of a fixed block effect. The proposed graphical method can be used as a useful tool for evaluating the effect of blocking in response surface designs with a fixed effect in terms of the prediction variance when the region of interest is cuboidal. That is, through the blocking effect graph, we can ascertain that which blocking arrangement minimizes the overall increase in the prediction variance, and compare the effect of blocking in the cases of orthogonal and non-orthogonal block designs, respectively, when a region of interest is cuboidal.

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

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