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Graphical Method for Evaluating the Prediction Variance Characteristics of Composite Mixed-Resolution Design

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Abstract: In this work, the prediction variance characteristics of the Composite Mixed-Resolution Designs (CMRD) were explored in spherical region using graphical procedures. Three-dimensional Variance Dispersion Graphs (VDG) was proposed and used as a graphical technique that assesses the designs' prediction capabilities. The replication of the cube and star portions of the CMRD as well as the centre point was considered in the evaluation of the designs. Under the spherical design region, the VDGs display the designs' prediction variances throughout the design region. The results show that replicating the star portion of the composite mixed-resolution designs for the practical axial distance, in most cases improves the scaled prediction variance property of the design.

Keywords: Axial distance, minimum aberration, noise factor, signal factor, variance dispersion graph

1 Introduction

Composite Mixed-Resolution Design (CMRD) is a response surface design developed by [1]. It allows the estimation of interaction and quadratic effects among controllable (signal) variables in the presence of noise variables. It is a response surface design which accommodates two set of factors, namely; the signal factors (x) and noise factors (z). Levels of signal factors can be easily to controlled in the process, whereas those of the noise factors cannot be controlled easily and are assumed to randomly vary within the process. In addition, it comprises three components: the factorial portion, the axial portion and the centre points.

The factorial portion is a 2^{K-p} full (p = 0) or fractional (p > 0) factorial mixed resolution design with *c* signal and *u* noise factors and with levels coded as ± 1 (where *K* is the number of factors and *p* is a positive integer). The factorial portion is a mixed-resolution design because it has at least Resolution *V* among the *c* signal factors, at least Resolution *III* among the *u* noise factors and none of the $c \times u$ signal-by-noise two-factor interactions are aliased with any main effect or any two-factor interaction. The axial portion consists of 2c star points. For each signal factor, the design includes two "star" points, i.e., the signal factor is set at levels $\pm \alpha$ and all other factors are set at mid-level 0. This means that the star points for the noise factors are excluded from the design. The n_0 centre points make up the third component of the design. The two parameters that must be specified for the design are the axial distance, α , of the star points from the centre of the design and the number of centre points, n_0 .

The present study adopts response surface methodology (RSM), which is a collection of mathematical and statistical techniques useful for the modeling and analysis of problems in which a response of interest is influenced by several variables and the objective is to optimize this response ([2]. Thus, a first-order model with interactions contains main effects and two-way interactions involving the control and noise factors and is given by

$$y_{ijkl} = \beta_0 + \sum_{i=1}^c \beta_i x_i + \sum_{k=1}^u \delta_k z_k + \sum_{i=1}^{c-1} \sum_{j=i+1}^c \beta_{ij} x_i x_j + \sum_{k=1}^{u-1} \sum_{l=k+1}^u \delta_{kl} z_k z_l + \sum_{i=1}^c \sum_{k=1}^u \delta_{ik} x_i z_k + e_{ijkl},$$
(1)

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where $\{x_i : i = 1, 2, ..., c\}$ and $\{z_k : k = 1, 2, ..., u\}$ are, respectively, the signal variables and the noise variables; y_{ijkl} is the response variable; the β 's and δ 's are, respectively, the signal and noise parameters, and ee_{ijkl} is the random error term.

Replication of experimental observations is indispensable for efficient and optimal performance of the second-order designs. Traditionally, the centre point of the design is replicated to ensure proper estimation of the experimental error with $n_0 - 1$ degrees-of-freedom because it is assumed that the optimum response is at the centre of the design. However, studies have shown that for the central composite design (CCD), replicating only at the centre may lead to estimating errors that may be too small for the correct evaluation of the model. There is no assurance that variability will remain constant throughout the design region. [3] posits that to replicate at other locations in the design region is sound experimental strategy. [4] used the variance dispersion graphs (VDG) to investigate the replication of the star component of the (CCD) for k = 5 and 6 factors. The study revealed that the overall performance of the scaled prediction variance (SPV) of the CCD is considerably improved by replicating the star points.

[1] developed the composite mixed-resolution designs through redefining Taguchi's model used in the Taguchi designs. That is, the designs are at least resolution V among the signal factors (i.e. among the *c* signal factors, no main effects or two-factor interactions are aliased with any other main-effect or two-factor interaction) and are at least resolution *III* among the noise factors. The experimental design region of interest in [1] is a hypercube. They also showed that the replication of the star points improves the *G*-efficiency of composite mixed resolution designs.

[5] addressed the performances of the partially-replicated cube and star (axial) portions of orthogonal central composite designs (CCD) in spherical regions using the variance dispersion graphs and fraction of design space plots as the two graphical techniques and the D- and G-efficiencies as the single-value criteria. Their results show that replicating the star portions of the CCD considerably reduces the prediction variance, thereby improving the G-efficiency in the spherical region. Hence, it was recommended for prediction with precision.

However, in this study, a function for plotting the variance dispersion graphs for the CMRD has been proposed. The presnrt study aims to obtain a graphical procedure, a three-dimensional variance dispersion graph, for evaluating the prediction variance characteristic of the composite mixed-resolution designs in spherical regions. The implications of replicating the cube and star portions of the CMRD on the distribution of SPV throughout the design region of interest is facilitated using $n_0 = 0, 1, 2, 3$ and 4 centre points.

2 Preliminaries

The concepts of design resolution and minimum aberration which are very vital in the development of the composite mixed-resolution designs are concisely discussed in this section.

2.1 Resolution

Resolution is a useful concept associated with 2^{K-p} fractional factorial designs. It is a criterion used in the selection of a fraction of important effects or effects of interest to the experimenter from a number of factor effects. A design is of resolution *R* if no *p*-factor effect is aliased with another effect containing less than R - p factors ([2]). In general, the resolution of a two-level fractional factorial design is equal to the number of letters in the shortest word in the defining relation. However, resolution is sometimes insufficient to distinguish between designs. Since designs with the same resolution may not be equally good, a more refined criterion, i.e. minimum aberration was introduced by [6].

2.2 Minimum Aberration

Minimum Aberration design is the design which minimizes the number of words in the defining relation of minimum length: see [6]. Let D_1 and D_2 be two m^{K-p} designs (where *m* is the level of the factors, *K* is the number of factors and *p* is the fraction of the factorial required) with v_{1u} and v_{2u} words of length u ($1 \le u \le K$). Let *r* be the smallest value of *u* for which $v_{1u} \ne v_{2u}$; then D_1 has less aberration than D_2 if $v_{1r} < v_{2r}$. If there exists no design with less aberration than D_1 , it has minimum aberration.



2.3 Variance Dispersion Graph

Variance Dispersion Graph (VDG) is a graphical tool introduced by [7] to evaluate the properties of the prediction variance of a design. It displays the scaled prediction variance (SPV) throughout a multi-dimensional region on a single two-dimensional graph (see [8]). At a point, x, in the design space, the scaled prediction variance is given by $NVar[\hat{y}(x)]/\sigma^2 = Nf'(x)(X'X)^{-1}f(x)$, where $Var[\hat{y}(x)]$ is the variance of predicted response, $\hat{y}(x)$, σ^2 is the unknown process variance, $f'(x) = [1, x_1, x_2, \dots, x_K; x_1^2, \dots, x_K^2; x_1x_2, \dots, x_{K-1}x_K]$, $(X'X)^{-1}$ is the inverse of the information matrix and X is the extended design matrix. The SPV is plotted against a radius, r, from the centre of the design space. The scaling is used to facilitate comparison among competing designs ([?]ontgomery). According to [?]i, desirable designs are those with the smallest SPV and reasonable stability in the design region. The benefits of SPV in model assessment have been widely acknowledged: see, for example, [7], [1], [10] and [9]. Often, the standardized or unscaled prediction variance (UPV), given by $Var[\hat{y}(x)]/\sigma^2 = f'(x)(X'X)^{-1}f(x)$ is preferred by some experimenters in design assessment (see, for example, [11]). Note that the difference between equations of the SPV and UPV is the number of runs in the design, N.

[9]state that the UPV is useful to compare designs of different sizes to define if the additional runs in a larger design substantially reduce the variance of the predicted response. They also allow for an estimate of the quality of prediction in absolute terms. SPV, on the other hand, allows the practitioner to measure the variance of the predicted response on a per observation basis and it penalizes larger designs over small designs. Scaling allows comparison of designs with different numbers of runs. The radius, *r* of a concentric ball or sphere is defined by [12] as $r = [\sum_{i=1}^{c} x_i^2]^{1/2} \Rightarrow r^2 = \sum_{i=1}^{c} x_i^2$. A design is considered to be good if it has low and stable SPV throughout the experimental region. A big gap between the maximum and minimum values implies that the variance function is unstable over the region ([13]). Comparisons among competing designs can be made easilyas well as the strength and weaknesses of the designs can be assessed using the VDG. This type of information would be difficult to be captured by single number criterion.

3 Model Development

The second-order model that allows for the estimation of the parameters associated with the CMRD is given by

$$y_{ijk} = \beta_0 + \sum_{i=1}^c \beta_i x_i + \sum_{k=1}^u \beta_{ii} x_i^2 + \sum_{i=1}^{c-1} \sum_{j=i+1}^c \beta_{ij} x_i x_j + \sum_{k=1}^{u-1} \delta_k z_k + \sum_{i=1}^c \Sigma_{k=1}^u \delta_{ik} x_i z_k + e_{ijk},$$
(2)

where y_{ijk} is the response variable, β 's and δ 's are the model parameters, x_i and z_k , respectively, are the signal and noise variables, and e_{ijk} is the random error term. The CMRD model excludes the interaction and quadratic effects of the noise variables which reduce the number of runs (because the axial portion of the noise variables is ignored) and thereby minimizing variability.

At a point, \mathbf{x} , in the design space, the prediction variance involving the signal and noise factors is given by

$$Var[\hat{y}(\mathbf{x},\mathbf{z})] = \sigma^2 \mathbf{x}^{\prime m} (X^{\prime} X)^{-1} \mathbf{x}^{m},$$

where $\mathbf{x}'^m = [1; x_1, \dots, x_c; x_1x_2, \dots, x_{c-1}x_c; x_1^2, \dots, x_c^2; z_1, \dots, z_u; x_1z_1, \dots, x_cz_u]$ is the vector of design points in the design space expanded to model form. Multiplying by *N* (the total number of runs) and dividing by σ^2 (the process variance), the resulting function,

$$\frac{NVar\left[\hat{y}(\mathbf{x},\mathbf{z})\right]}{\sigma^2} = N\mathbf{x}'^m (X'X)^{-1} \mathbf{x}^m,\tag{4}$$

is the scaled prediction variance (SPV). The closed form of the scaled prediction variance was developed in this study for evaluating the performances of the CMRD.

4 Methodology

4.1 Design Considerations

The nine designs used in this study were taken from the table of Minimum Aberration Mixed Resolution (MAMR) designs in [4] for factors K = 4 to 8. Therefore, the generators of the designs used in this work are given in Table 1. The designs

(3)

Design	Κ	SF	NF	Fraction	SFR	NFR	Generator(s)/Defining relation(s)
1	4	AB	CD	2^{4}	_	_	—
2	5	ABC	D(E)	2^{5-1}	V	V	E = ABCD
3	6	ABCD	E(F)	2^{6-1}	IV	IV	F = ABCDE
4	7	ABC	DE(FG)	2^{7-2}	V	IV	F = ABCE, G = ABCD, DEFG
5	7	ABCD	E(FG)	2^{7-2}	V	III	F = ABCD, G = ABCDE, EFG
6	7	ABCDE	F(G)	2^{7-1}	VII	VII	G = ABCDEF
7	8	AB	CDE(FGH)	2^{8-3}	V	IV	F = ABCE, G = ABCD, H = ABDE
							DEFG, CDFH, CEGH, ABFGH
8	8	ABC	DE(FGH)	2^{8-3}	V	III	F = ABCE, G = ABCD, H = ABCDE
							DEFG, EGH, DFH, ABCFGH
9	8	ABCDEF	GH	2^{8-2}	V	V	G = CDEF, H = ABEF, ABCDGH

Table 1: Generators of MAMR Designs

are labeled according to the total number of design factors, K = 4, ..., 8 and reference letters, A, B, ..., H. A generator (e.g. E = ABCD) is a set of columns (representing some factors) used to generate other factors that are not present in the fraction. For instance, for design 2, the fractional factorial required for the designs is 2^{5-1} . Therefore, 5 - 1 = 4 factors (*ABCD*) is generated normally but the remaining factor (*E*) is generated with the generator (E = ABCD) by multiplying the *ABCD* columns together to achieve the *E* column. The letters in the "Signal factors" and "Noise factors" columns (excluding the letters in bracket), correspond to the K - p columns generated using the full factorial design in K - p factors. The levels of the remaining *p* factors (letters in the bracket) are generated using the *p* generators in the last column of Table 1. For example, Design 4 has c = 3 signal factors and u = 4 noise factors. The factors (*ABCDE*) is generated normally while the levels of the remaining p = 2 factors (*FG*) is generated using the two generators (*F = ABCE*, *G = ABCD*). Simply, SF, NF, SFR and NFR in Table 1, respectively, denote Signal Factors, Noise Factors, Signal Factor Resolution and Noise Factor Resolution.

To facilitate the evaluation of the designs using the graphical method, the cube and star replications of the CMRD were adopted. For each replication of the cube portion, the star portion is not replicated and for each replication of the star portion, the cube portion is not replicated. Five versions of the designs are generated through replicating the cube and star portions by different amount. The first design is where the cube and star were not replicated. This design is denoted by C1S1. The second is C1S2, where the star is replicated twice and the cube is not replicated. Other designs are generated for each of the second-order CMRD designs for the K = 4 to 8 factors under consideration.

In the spherical design region, the spherical and practical axial distances, $\alpha = \sqrt{K}$ and $\alpha = K^{1/4}$, respectively, were considered in the evaluation of the CMRD, where K = c + u is the number of experimental factors. The practical α was proposed by [14] as compromise between the spherical and cuboidal axial distances. The cuboidal axial distance is given by $\alpha = 1$ which defines the cuboidal region. It has been observed by [9] that placing the axial runs at practical α levels results in stability of the estimated parameters which yields gain in prediction precision. The practical α is very useful especially when the number of factors is large (K > 5) as it provides design points that are less extreme.

4.2 Prediction Variance for the VDG

An expression for the unscaled prediction variance function, $UPV = \mathbf{x}'^m (X'X)^{-1} \mathbf{x}^m$, was obtained by determining the information matrix, X'X, its inverse, $(X'X)^{-1}$, and then pre- and post-multiplying the inverse by \mathbf{x}'^m and \mathbf{x}^m , respectively. Now, for Design 2 in Table 1, with the following properties:

–Number of factors, K = 5

-Fraction= 2^{5-1}

-Signal/Noise factors Resolution = 5

-Shperical $\alpha = 2.236$

- -Signal factors (c = 3):A, B, C
- -Noise factors (u = 2):D, E
- -Defining relation: A, B, C, D, E

The extended design matrix of the composite mixed-resolution design obtained from the model in equation (2) is given by, X, while the information matrix is X'X. Let t be the number of replication of the star, n, the number of replication of the cube and F = nf, where f is the size of the factorial component. Then, taking cue from [4], the block form of the information matrix is given by

$$\begin{bmatrix} N & \phi_c' & (F+2t\alpha^2).j' & \phi_m' \\ \phi_c & diag(d_i) & \theta_1' & \theta_2' \\ (F+2t\alpha^2).j & \theta_1 & [(2t\alpha^4)I_c+F.J_c] & \theta_2' \\ \phi_m & \theta_2 & \theta_2 & F.I_m \end{bmatrix}$$

while the block form of the inverse of the information matrix is given as

$$\begin{bmatrix} \lambda_1 & \phi_c' & \lambda_2.j' & \phi_m' \\ \phi_c & diag(1/d_i) & \theta_1' & \theta_2' \\ \lambda_2.j & \theta_1 & -\frac{1}{T} \left\{ (2N\alpha^4 t).I_c - \lambda_3[c.I_c - J_c] \right\} & \theta_2' \\ \phi_m & \theta_2 & \theta_2 & (1/F).I_m \end{bmatrix}$$

where $\phi_c = c \times 1$ zero vector, $\theta'_1 = c \times c$ zero matrix, $\theta_2 = m \times c$ zero matrix, $m = \binom{c}{2}u + cu$, $j = c \times 1$ unit vector, $I_c = c \times c$ identity matrix, $diag(d_i) = c \times c$ diagonal matrix such that $d_i = F + 2t\alpha^2$ for $1 \le i \le c$, $I_m = m \times m$ diagonal matrix, $T = 8c\alpha^8 t^3 - 8c\alpha^6 F t^2 - 4N\alpha^8 t^2 + 2c\alpha^4 F^2 t - 2cN\alpha^4 F t$, $\lambda_1 = \frac{-(2t\alpha^4 + cF)}{Q}$, $\lambda_2 = \frac{2t\alpha^2 + F}{Q}$, $\lambda_3 = F^2 - NF + 4\alpha^4 t^2 + 4\alpha^2 F$, and $Q = cF^2 - cNF + 4c\alpha^4 t^2 - 2N\alpha^4 t + 4c\alpha^2 F t$.

Pre- and post-multiplying the information matrix by $\mathbf{x}^{\prime m}$ and \mathbf{x}^{m} , the general closed form of the prediction variance for the composite mixed-resolution design (CMRD) is given by

$$V(\mathbf{x}, \mathbf{z}) = \left\{\frac{(c-1)\lambda_3 - \omega}{T}\right\} \sum_{i=1}^{c} x_i^4 + \left\{\frac{1}{F} - \frac{2\lambda_3}{T}\right\} \sum_{i(5)$$

where $\Delta = F + 2t\alpha^2$ and $\omega = 2N\alpha^4 t$. The scaled prediction variance (SPV) is

$$V(\mathbf{x}, \mathbf{z}) = N \left\{ A \sum_{i}^{c} x_{i}^{4} + B \sum_{i < j}^{c} x_{i}^{2} x_{j}^{2} \sum_{i}^{c} x_{i}^{2} + D[\sum_{k}^{u} z_{k}^{2} + \sum_{i}^{c} \sum_{k}^{u} x_{i}^{2} z_{k}^{2}] + E \right\}$$
(6)

where $A = \frac{(c-1)\lambda_3 - \omega}{T}$, $B = \frac{1}{F} - \frac{2\lambda_3}{T}$, $C = \lambda_2 + \frac{1}{A}$, $D = \frac{1}{F}$ and $E = \lambda_1$. To obtain the prediction variance for the variance dispersion graph, maximize $V(\mathbf{x}, \mathbf{z})$ subject to $r^2 = \sum_{i=1}^{c} x_i^2 + \sum_{k=1}^{u} z_k^2$. Without loss of generality, the constraint can be expressed as $r^2 = r_x^2 + r_z^2$, where $r_x^2 = \sum_{i=1}^{c} x_i^2$ and $r_z^2 = \sum_{k=1}^{u} z_k^2$, corresponding to the signal and noise factors, respectively. Substituting r_x^2 and r_z^2 into Equation (6), the general form of the scaled prediction variance may be simplified to

$$V(\mathbf{x}, \mathbf{z}) = N \left\{ A \sum_{i}^{c} x_{i}^{4} + Br_{x}^{4} + Cr_{x}^{2} + Dr_{z}^{2}(1 + r_{x}^{2}) + E \right\}$$
(7)

Consequently, the problem of evaluating $V(\mathbf{x}, \mathbf{z})$ on a sphere of radius, r, reduces to the problem of evaluating $\sum_{i=1}^{c} x_{i}^{4}$ subject to $\sum_{i}^{c} x_{i}^{2}$. In order to solve this problem, the principle of Lagrangian multipliers is used to find the critical points which analytically define the minimum (*Vminr*) value for the prediction variance at radius, r. Therefore, $\sum_{i}^{c} x_{i}^{4} = r_{x}^{2}/c$ (see [4] and [15]) and the SPV function becomes

$$V(\mathbf{x}, \mathbf{z}) = N\left\{ (A + Bc)\frac{r_x^4}{c} + Br_x^4 + Cr_x^2 + Dr_z^2(1 + r_x^2) + E \right\}$$
(8)

This function was used in plotting the variance dispersion graphs for the evaluation of the prediction variance performances of the composite mixed resolution designs.



Figure 1: Design 1 with Spherical Alpha at $n_0=4$



Figure 2: Design 2 with Spherical Alpha at $n_0=4$

5 Design Evaluation and Comparison

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In this section, variance dispersion graphs were plotted from the scaled prediction variance function developed herein. The scaled prediction variances were computed and the results were plotted against the radii $0 \le r_x \le 1$ and $0 \le r_z \le 1$. The SPV are plotted on the y-axis, while the radii are plotted on the x-axis. The variance dispersion graphs were plotted for $n_0 = 0, 1, 2, 3$ and 4 centre points, but only the graphs for $n_0 = 4$ were presented for simplicity and clarity for the spherical and practical axial distances.

With spherical axial distance, star replicated designs with $n_0 = 0, 1$ and 2 centre points have the lowest prediction variances. The exceptions are Design 2 where replicating the cube twice (*C2S1*) displays the lowest SPV and also Designs 1, 2 and 3 where non-replication of the cube and star (*C1S1*) reflects the lowest SPV. For the designs with $n_0 = 3$ and 4 centre points, *C1S1* reveals the lowest SPV throughout the design region. The graphs for the spherical axial distance with four centre points are indicated in Figures 1 - 9. Thus, we can conclude that when the axial distance is spherical, replication of the star with $n_0 = 0, 1$ and 2 centre points offers minimum scaled prediction variance. However, with higher number of centre points, $n_0 = 3$ and 4, *C1S1* is superior to the other design options in terms of minimum SPV. On the other hand, the designs with the largest scaled prediction variance are the designs with their cube portions replicated.



Figure 4: Design 4 with Spherical Alpha at $n_0=4$

For the practical axial distance, SPV does not exist for C1S1, C1S2 and C1S3 options of Design 1. For the remaining design options, the variance dispersion graphs are displayed in Figures 10 to 18 for Designs 1 to 9 with practical axial distances and four centre points. The VDGs reveal that the designs with star replication have the lowest SPV for most of the designs over the entire design space at different values of the centre points. We note from the plots of designs with practical α that for all the centre points considered, the designs with the highest prediction variance are the designs where the cube portion is replicated thrice (C3S1).



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Figure 5: Design 5 with Spherical Alpha at $n_0\!\!=\!\!4_{\&}$



Figure 6: Design 6 with Spherical Alpha at $n_0=4$



Figure 7: Design 7 with Spherical Alpha at $n_{0}\!\!=\!\!4$



Figure 8: Design 8 with Spherical Alpha at $n_0=4$



Figure 9: Design 9 with Spherical Alpha at $n_0=4$

6 Conclusion

The results exhibit that increase in centre points affects the performance of the designs. We can conclude that for designs with spherical α , the best designs are those without replication of cube or star portion (*C*1*S*1). But for the designs with practical α , most of the VDG plots show that the replication of star portion substantially lead to minimum spread of the scaled prediction variance throughout the entire design region. Moreover, VDG plots illustrate that replication of the cube portion of the designs produced the highest prediction variance on most of the graphs. Thus, it is not recommended.



Figure 10: Design 1 with Practical Alpha at $n_0=4$



Figure 11: Design 2 with Practical Alpha at $n_0=4$



Figure 12: Design 3 with Practical Alpha at $n_{0}\!\!=\!\!4$



Figure 13: Design 4 with Practical Alpha at $n_0=4$



Figure 14: Design 5 with Practical Alpha at $n_0=4$



Figure 15: Design 6 with Practical Alpha at $n_0=4$



Figure 16: Design 7 with Practical Alpha at $n_0=4$



Figure 17: Design 8 with Practical Alpha at $n_0=4$







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