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A Study on the Influence of a Missing Cell in a Class of Central Composite Designs †

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ABSTRACT

The central composite design is widely used in the response surface analysis, because it can fit the second order model with small experimental points. In practice, the experimental data are not always obtained on all the points. When there are missing observations, many problems due to the missing cells can occur. In this paper, the influence of a missing cell on the central composite design is discussed. First, the influences of a missing cell on the variances of estimated regression coefficients are compared as α varies. Second, how the average prediction variance is affected by a missing sell is discussed. And the influence on rotatability is investigated. Third, the influence of a missing cell on optimality, especially on D-optimality and A-optimality, is examined.

Key Words : central composite design, missing cell, average prediction variance, rotatability, D-optimality, A-optimality.

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1. INTRODUCTION

In these days, many statistical methods are being used in various fields. Especially, experimental design method is very important to engineers, chemists, biologists, and so on. The Central Composite Design(CCD) is one of designs which are being used widely. The CCD has been studied by many statisticians in Response Surface Analysis. Myers and Montgomery(1995) discussed the efficiency of experimental designs, and compared CCD with the other designs on D-, A-, G-, or Q-optimality. Yandell(1995) investigated the method of analysis for designed experiment when there are missing cells. Box and Draper(1963) suggested several criteria which can be used in the selection of design. Park, Lim and Baba(1993) suggested a measure of rotatability that enables us to assess the degree of rotatability for a given design. Hader and Park(1978) discussed about slope-rotatable central composite designs. Lucas(1974) investigated D-efficiency and G-efficiency in central composite design.

In this paper, the effect of elimination of a missing cell in CCD will be discussed. In CCD, experimenter can choose any value of $\alpha > 0$ in the design. For example, one can take $\sqrt{2}$ for α so that the design has rotatability when two factors are considered.

In Section 2, it will be discussed how the value of α affects the variances of estimators of regression coefficients when there is a missing observation. It is almost impossible to obtain the analytic solution of α which supports the minimum variances of estimators of regression coefficients. In Section 3, the influence of a missing cell on the average prediction variance and rotatability will be examined. In Section 4, the influence of a missing cell on optimality will be discussed. D- and A-optimality will be compared respectively when there is a missing observation on the center point, factorial point, or axial point.

2. COMPARISON OF VARIANCES OF ESTIMATED REGRESSION COEFFICIENTS WHEN A MISSING CELL EXISTS

2.1. Model and covariance matrix of CCD

Consider the second order model when there are two independent variables. The model is given as follows ;

$$y(\boldsymbol{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} {x_1}^2 + \beta_{22} {x_2}^2 + \beta_{12} x_1 x_2 + \epsilon \tag{1}$$

where ϵ is independently and normally distributed with zero mean and variance σ^2.

In CCD with two variables, the experimental points are composed of four factorial points, center points and four axial points. So the number of design points is 9 if one center point is used in the design. The design matrix and covariance matrix of estimators of regression coefficients for model (1), containing one center point, are

$$X = \begin{array}{c} \\ \end{array} \overset{\begin{array}{cccccc} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{array}}{\begin{pmatrix} 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & \alpha & 0 & \alpha^2 & 0 & 0 \\ 1 & -\alpha & 0 & \alpha^2 & 0 & 0 \\ 1 & 0 & \alpha & 0 & \alpha^2 & 0 \\ 1 & 0 & -\alpha & 0 & \alpha^2 & 0 \end{pmatrix}}$$

$$(X'X)^{-1}\sigma^2 = \begin{pmatrix} 9 & 0 & 0 & 4+2\alpha^2 & 4+2\alpha^2 & 0 \\ & 4+2\alpha^2 & 0 & 0 & 0 & 0 \\ & & 4+2\alpha^2 & 0 & 0 & 0 \\ & & & 4+2\alpha^4 & 4 & 0 \\ & symm. & & & 4+2\alpha^4 & 0 \\ & & & & & 4 \end{pmatrix}^{-1} \sigma^2$$

2.2. When a missing cell exists in CCD

Experiments may run into problem during implementation. Animals or patients may die or be taken off study, materials may be accidentally destroyed, or data misrecorded in the ways that cannot be later deciphered. In these cases, it is necessary to analyze the data excluding the missing observation. If the observation on $(\alpha, 0)$ is missing, elimination of the missing cell reduces the design matrix and the covariance matrix given in the previous section as follows ;

$$X = \begin{pmatrix} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -\alpha & 0 & \alpha^2 & 0 & 0 \\ 1 & 0 & \alpha & 0 & \alpha^2 & 0 \\ 1 & 0 & -\alpha & 0 & \alpha^2 & 0 \end{pmatrix}$$

$$(X'X)^{-1}\sigma^2 = \begin{pmatrix} 8 & -\alpha & 0 & 4+\alpha^2 & 4+2\alpha^2 & 0 \\ & 4+\alpha^2 & 0 & -\alpha^3 & 0 & 0 \\ & & 4+2\alpha^2 & 0 & 0 & 0 \\ & & & 4+\alpha^4 & 4 & 0 \\ & symm. & & & 4+2\alpha^4 & 0 \\ & & & & & 4 \end{pmatrix}^{-1} \sigma^2$$

To compute the exact covariance matrix is not difficult if a mathematical package can be used, but not so helpful to understand the structure. So the graph of variances versus the value of α will be shown.

Without loss of generality, we may assume $\sigma^2 = 1$. Figures 2-1 through 2-6 show the change of variances of estimated regression coefficients as the value of α varies. Each graph has three curves, the numbered 1 curve is for full points (the case that there are no missing cells), the numbered 2 curve is for the case that the factorial point (1, 1) is the missing cell, the numbered 3 curve is for the case that the axial point $(\alpha, 0)$ is the missing cell. The other case like $(0, \alpha)$ missing is the same to the case of $(\alpha, 0)$ missing, except the role of $\mathrm{Var}(\hat{\beta}_1)$ is exchanged by that of $\mathrm{Var}(\hat{\beta}_2)$ and the role of $\mathrm{Var}(\hat{\beta}_{11})$ is exchanged by that of $\mathrm{Var}(\hat{\beta}_{22})$. The other cases can be thought similarly. The case of missing on the center point is not analyzed, since the $X'X$ is not so much changed (only the value of (1,1) element is changed from 9 to 8), when the center point is missing.

In Figure 2-1, we can see that variance of $\hat{\beta}_0$ is not so much influenced whether there is a missing cell or not. In Figures 2-2, 2-3 and 2-6, the variances of estimator are quite different when the factorial point (1, 1) is missing. Especially, the influence of missing factorial point is very serious when α is less than 1, and stabilized when α is larger than 1.

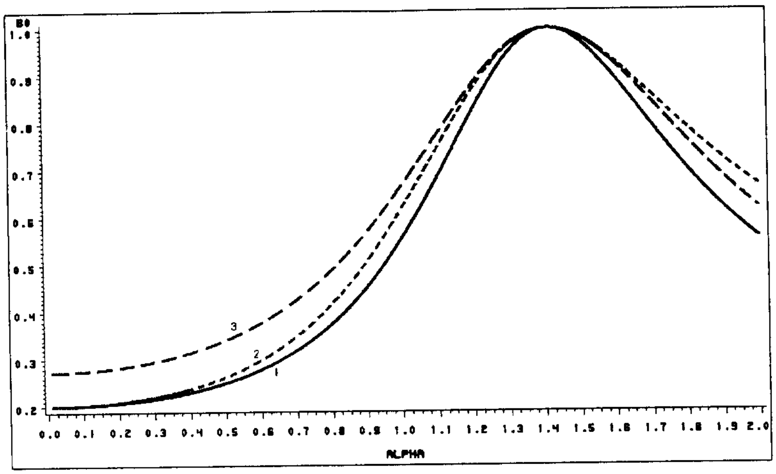

Figure 2-1. variance of $\hat{\beta}_0$

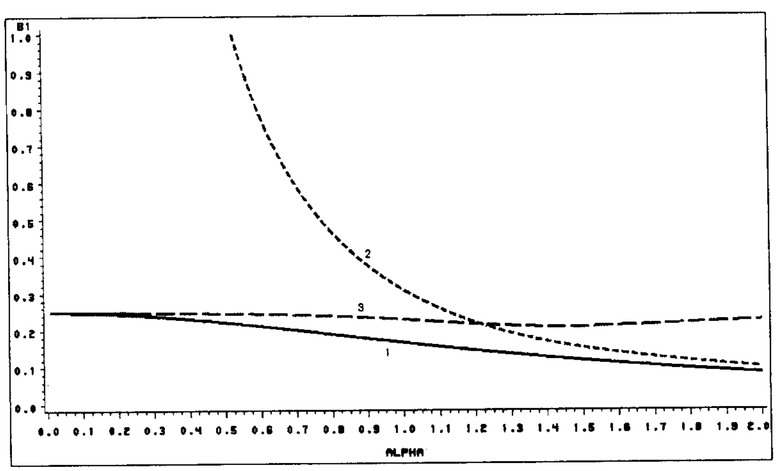

Figure 2-2. variance of $\hat{\beta}_1$

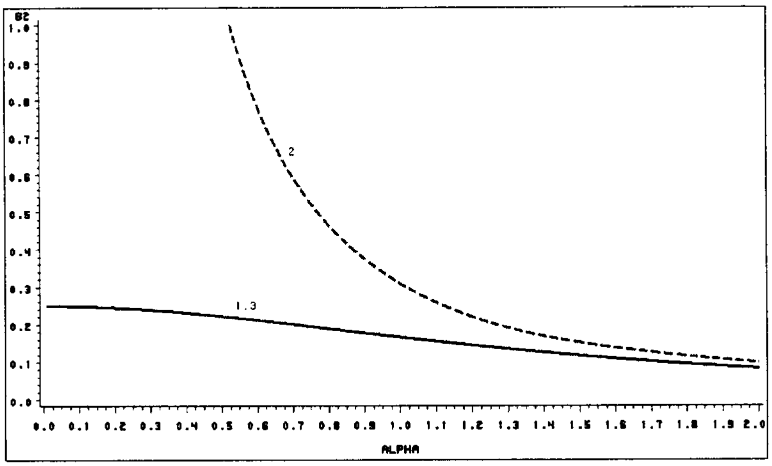

Figure 2-3. variance of $\hat{\beta}_2$

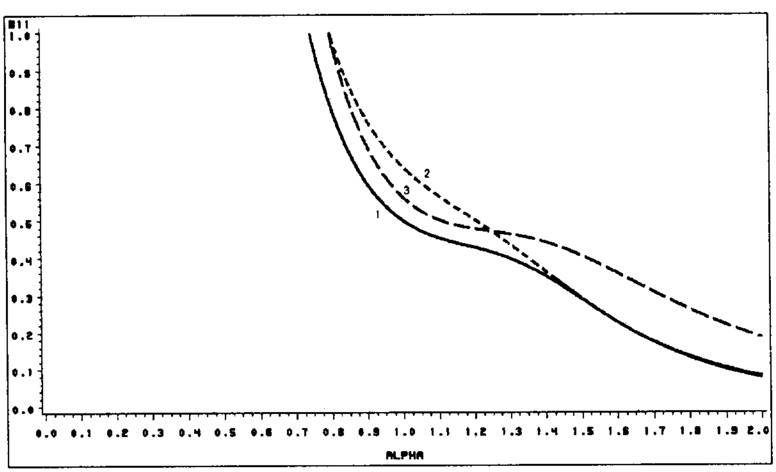

Figure 2-4. variance of $\hat{\beta}_{11}$

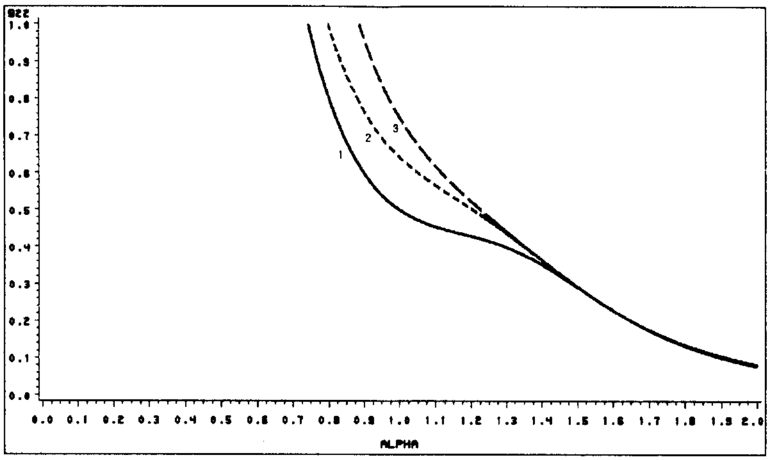

Figure 2-5. variance of $\hat{\beta}_{22}$

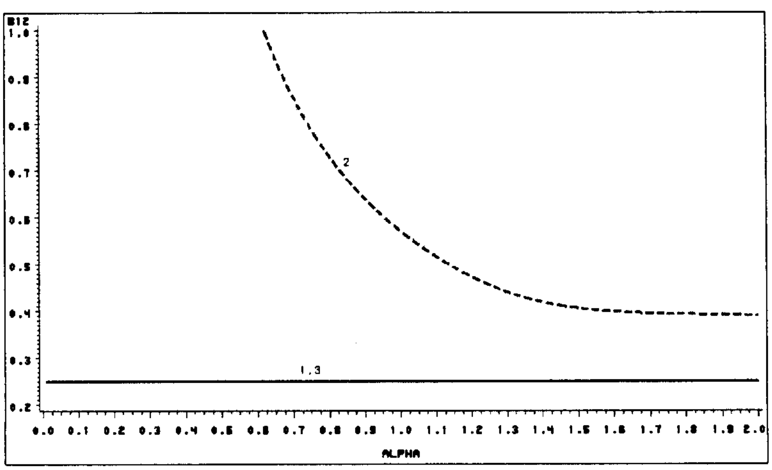

Figure 2-6. variance of $\hat{\beta}_{12}$

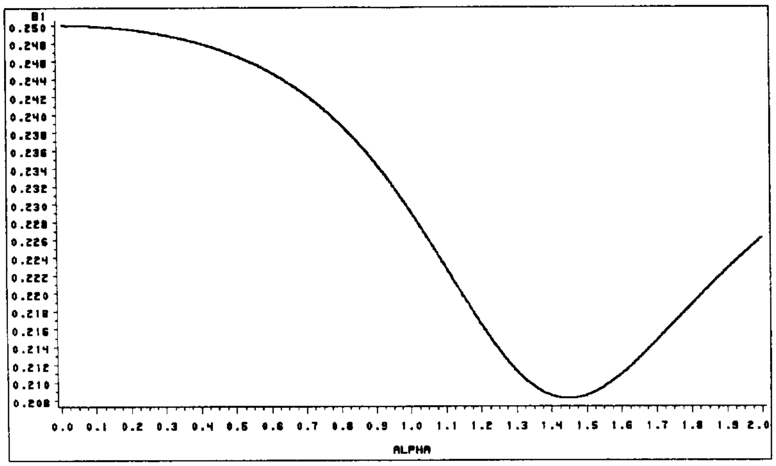

Figure 2-7. $\mathrm{Var}(\hat{\beta}_1)$ when $(\alpha, 0)$ is the missing cell

In case of the axial point $(\alpha, 0)$ missing, the variances of $\hat{\beta}_2$ and $\hat{\beta}_{12}$ are the same to those of the case which has no missing cell (Figures 2-3 and 2-6). But the variance of $\hat{\beta}_1$ differs more and more with that of the case which has no missing cell, as α increases. Figure 2-7 is a magnification of variance of $\hat{\beta}_1$ alone, in case of $(\alpha, 0)$ missing . When α is about 1.4 , the variance of $\hat{\beta}_1$ is minimized to about 0.208.

In Figure 2-7, we can see that $\mathrm{Var}(\hat{\beta}_1)$ decreases when α is less than about 1.4, and increase when α is greater than that. The value of α which makes $\mathrm{Var}(\hat{\beta}_1)$ be minimized is 1.4485. In Figures 2-4 and 2-5, the value of α which is less than 1 is not recommendable, since $\mathrm{Var}(\hat{\beta}_{11})$ and $\mathrm{Var}(\hat{\beta}_{22})$ become too large.

To summarize, the value bigger than about 1.4 is preferable for α in sense of variance minimization, and this region of α makes the design robust to the existence of a missing cell. As the value of α increases, the variances of estimators decrease. But the variance of a certain estimator increases as α does when there is a missing cell. So the value of α can be taken in each experiment, but the experimenter should know that the value less than 1.4 is not so preferable.

2.3. CCD with more variables or center points

In the previous section, CCD with two variables and one center point was discussed. Now consider the design which has more variables or center points.

The results are very similar to the previous case, but the value of α which minimizes $\mathrm{Var}(\hat{\beta}_1)$ in the case of $(\alpha, 0)$ missing is changed.

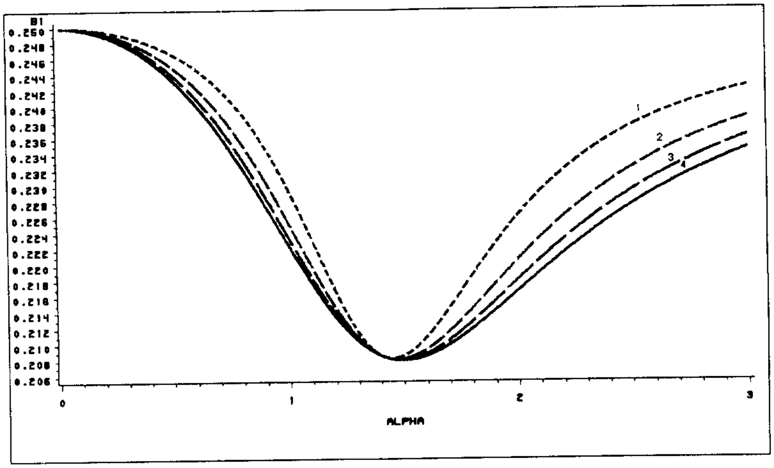

Figure 2-8. $\mathrm{Var}(\hat{\beta}_1)$ when $(\alpha, 0)$ is missing (two variables)

Figures 2-8, 2-9 and 2-10 show the change of α which minimizes $\mathrm{Var}(\hat{\beta}_1)$ in the case of $(\alpha, 0)$ missing. Figure 2-8 is for the case of two variables, Figures 2-9 and 2-10 are for three and four variables each. Each graph has four curves, and the numbers written on curves are the number of center points.

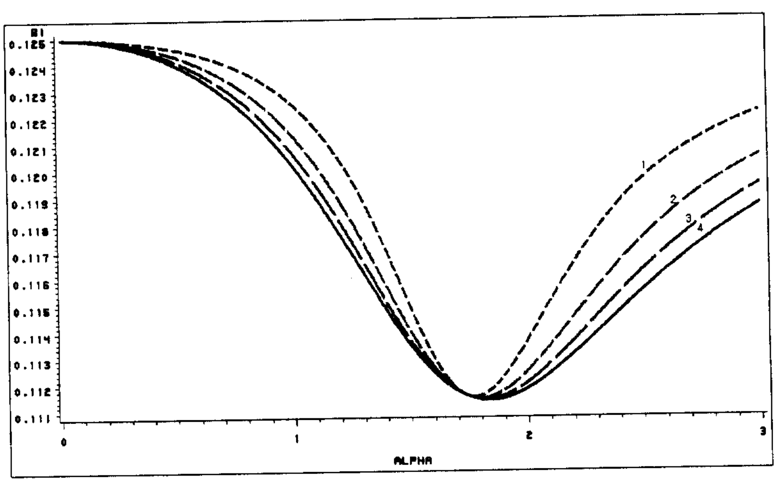

Figure 2-9. $\mathrm{Var}(\hat{\beta}_1)$ when $(\alpha, 0)$ is missing (three variables)

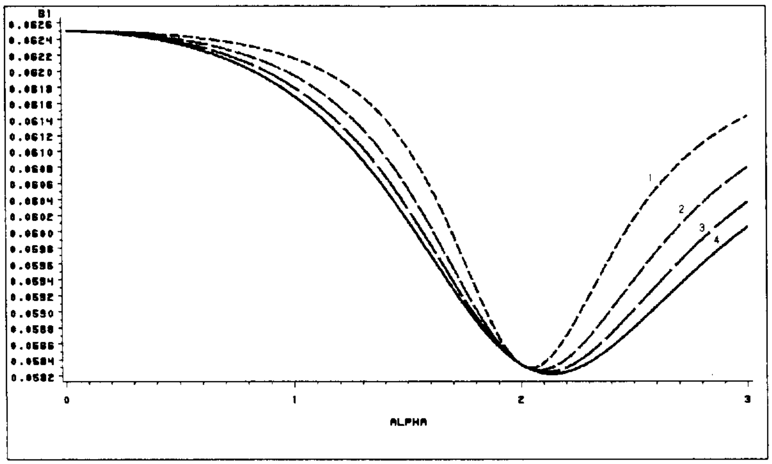

Figure 2-10. $\mathrm{Var}(\hat{\beta}_1)$ when $(\alpha, 0)$ is missing (four variables)

In Figures 2-8, 2-9 and 2-10, we can see that as the number of center points increases, the value of α which minimizes $\mathrm{Var}(\hat{\beta}_1)$ in the case of $(\alpha, 0)$ missing increases. And for the same number of center points, the value of α which minimizes $\mathrm{Var}(\hat{\beta}_1)$ also increases as the number of variables increases.

3. COMPARISON OF AVERAGE PREDICTION VARIANCE AND ROTATABILITY WHEN A MISSING CELL EXISTS

3.1. Comparison of Average Prediction Variance

Box and Draper(1963) suggested the use of an average mean squared error(AMSE), where the quantity $E[\hat{y}(\underline{x}) - f(\underline{x})]^2$ is averaged over $\underline{x}$ in a preselected region of interest. Here $f(\underline{x})$ is the true functional relationship between the dependent variable and the independent variables. In other words, a quantity

$$AMSE = \frac{NK}{\sigma^2} \int_R E[\hat{y}(\underline{x}) - f(\underline{x})]^2 d\underline{x}$$

was suggested where N is the total number of observations, R is the region of interest and $K = 1/\int_R d\underline{x}$. The $AMSE$ can be subdivided as follows ;

$$\begin{aligned} AMSE &= \frac{NK}{\sigma^2}\int_R E[\hat{y}(\underline{x}) - E\hat{y}(\underline{x})]^2 d\underline{x} + \frac{NK}{\sigma^2}\int_R [E\hat{y}(\underline{x}) - f(\underline{x})]^2 d\underline{x} \\ &= APV + ASB \end{aligned}$$

where APV stands for average prediction variance and ASB stands for average squared bias.

In this section, APV will be compared with one another when there is a missing cell. Note that APV can be written as follows

$$APV = \frac{NK}{\sigma^2}\int_R Var(\hat{y}(\underline{x}))d\underline{x}$$

Consider CCD with two variables and one center point. If the region of interest is $R = \{(x_1, x_2)| -1 \le x_i \le 1, i = 1, 2\}$, then $K = 1/4$. Then APV can be computed with the following equation.

$$APV = \frac{N}{4}\int_{-1}^{1}\int_{-1}^{1} \underline{x}'(X'X)^{-1}\underline{x}dx_1 dx_2$$

The APV is affected by the missing cell. And, the influence of the missing cell on the APV is quite different according to the point where the missing occurs. The results of computation as α varies are given in Figure 3-1.

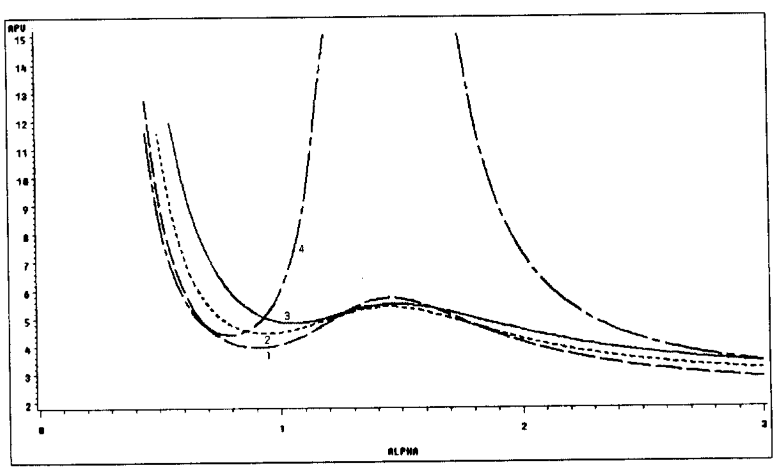

Figure 3-1. APV when missing cell exists

There are four curves in Figure 3-1. Numbered 1 curve is for the case of no missing, 2 is for the missing on the axial point, 3 is for the missing on the factorial point, and 4 is for the missing on the center point. It shows that the missing on the factorial or axial point has a little effect on *APV*. But the missing on the center point has a bad effect on *APV* when the value of α lies between 1 and 2. In any case, α less than 0.5 is not preferable in the sense of *APV*. The CCD with more variables or center points can be examined similarly.

3.2. A measure of rotatability

Park, Lim and Baba(1993) suggested a measure of rotatability. Let

$$V(\underline{x}) = \frac{N}{\sigma^2} Var(\hat{y}(\underline{x}))$$

where $\mathrm{Var}(\hat{y}(\underline{x})) = \underline{x}'(X'X)^{-1}\underline{x}\sigma^2$. In the $k-$dimensional space ($k \geq 2$), $V(\underline{x})$ can be expressed in terms of spherical coordinates of $(\rho, \phi_1, \cdots, \phi_k - 2, \theta)$, where

$$\begin{aligned}
x_1 &= \rho \cos\phi_1, \\
x_2 &= \rho \sin\phi_1 \cos\phi_2, \\
&\vdots \\
x_{k-1} &= \rho \sin\phi_1 \sin\phi_2 \cdots \sin\phi_{k-2} \cos\theta, \\
x_k &= \rho \sin\phi_1 \sin\phi_2 \cdots \sin\phi_{k-2} \sin\theta,
\end{aligned}$$

and

$$\rho \geq 0, 0 \leq \phi_1, \cdots, \phi_{k-2} \leq \pi, 0 \leq \theta < 2\pi.$$

Then $V(\underline{x})$ can be expressed as a function of $\rho, \phi_1, \cdots, \phi_{k-2}, \theta$. i.e. $V(\underline{x}) = \omega(\rho, \phi_1, \cdots, \phi_{k-2}, \theta)$. Let

$$\bar{\omega}(\rho) = \frac{1}{I_k} \int_0^{2\pi} \int_0^{\pi} \cdots \int_0^{\pi} \omega(\rho, \phi_1, \cdots, \phi_{k-2}, \theta) d\Omega$$

where $d\Omega = \sin^{k-2}\phi_1 \cdots \sin\phi_{k-2} d\phi_1 \cdots d\phi_{k-2} d\theta$, and

$$I_k = \int_0^{2\pi} \int_0^{\pi} \cdots \int_0^{\pi} d\Omega = \frac{2\pi^{\frac{k}{2}}}{\Gamma(\frac{k}{2})}.$$

$\bar{\omega}(\rho)$ means the averaged value of $V(\underline{x})$ over all the points on the hypersphere of radius ρ centered at the origin.

To be rotatable,

$$\omega(\rho, \phi_1, \cdots, \phi_{k-2}, \theta) = \bar{\omega}(\rho) \qquad \text{for all } \rho, \phi_i, \theta.$$

For a given design, the discrepancy from rotatability at ρ can be expressed as

$$h(\rho) = \int_0^{2\pi} \int_0^{\pi} \cdots \int_0^{\pi} [\omega(\rho, \phi_1, \cdots, \phi_{k-2}, \theta) - \bar{\omega}(\rho)]^2 d\Omega.$$

If the region of interest is $0 \leq \rho \leq 1$, the measure is

$$P_k(D) = \frac{1}{1 + R_k(D)}$$

where $R_k(D) = \frac{1}{E_k} \int_0^1 \rho^{k-1} h(\rho) d\rho$, and E_k is a positive constant depending only on k.

Let us take E_k to be

$$E_k = \int_0^1 \rho^{k-1} I_k d\rho = \frac{1}{kI_k}$$

for convenience.

$R_k(D)$ represents the average of $(\omega - \bar{\omega})^2$ over the region of integration. $P_k(D)$ is 1 if and only if a design is rotatable, and it is smaller than one for a nonrotatable design.

3.3. Influence of a missing cell on rotatability

Consider CCD with two variables and one center point. In this case, the two variables can be transformed as follows ;

$$x_1 = \rho \cos\theta,\ x_2 = \rho \sin\theta, \text{ where } \rho \geq 0, 0 \leq \theta < 2\pi.$$

Then the measure of rotatability can be computed as described in Section 3.2.

The result is given in Figure 3-2 when the region of interest is $0 \leq \rho \leq 1$. Each curve is obtained by calculating $P_k(D)$ as α varies. The numbered 1 curve is for no missing case, 2 is for the missing on the axial point, 3 is for the missing on the factorial point, and 4 is for the missing on the center point.

As the curve 4 shows, missing of the center point is not so influential on rotatability. Curves 2 and 3 show that missing on the factorial or axial point has bad effect on rotatability. However, depending upon the value of α selected, the effect of each point on rotatability is changed.

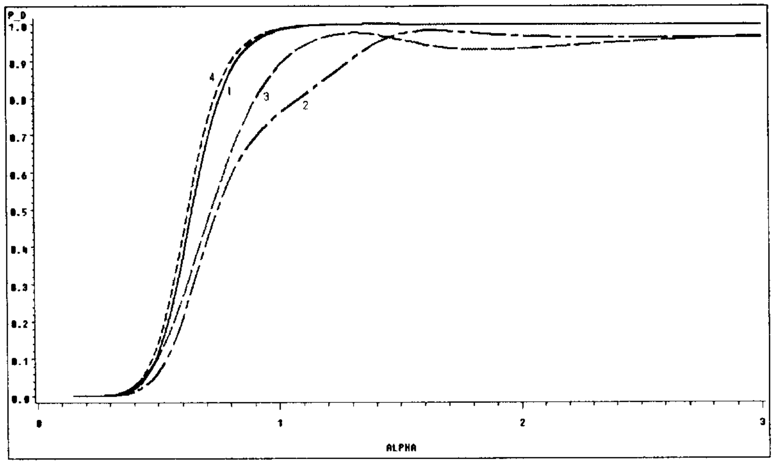

Figure 3-2. $P_k(D)$ when missing cell exists

4. COMPARISON IN THE SENSE OF D- AND A- OPTIMALITY

4.1. D-Optimality

D-Optimality is based on the notion that the experimental design should be chosen so as to achieve certain properties in the moment matrix

$$M = \frac{X'X}{N}$$

It is well known that the inverse of M, namely

$$M^{-1} = N(X'X)^{-1}$$

contains variances and covariances of the regression coefficients, scaled by N/σ^2. As a result, control of the moment matrix by design implies control of the variances and covariances.

The D-optimal design is one in which $|M| = |X'X|/N^p$ is maximized, where p is the number of parameters in the model. Nalimov, Golikova and Mikeshina(1970) studied on practical use of D-optimality. In Section 4-2, the determinants of M's will be compared as α varies, and that of missing cases will be discussed.

4.2. Influence of a missing cell on D-Optimality

In CCD the determinant of moment matrix defined in the previous section has a tendency of increase as α increases. That is, a larger value of α is recommendable for D-optimal sense. But in practical experiment, the region of interest is usually restricted and the conditions of experiment cannot be set for a large α. So, it is necessary for the experimenter to choose α as large as possible in the controllable region of interest.

Now, consider the existence of a missing cell. The determinant of moment matrix will be affected by a missing cell.

Figure 4-1 has four curves of determinant of moment matrix in the CCD which has two variables and one center point. Numbered 1 curve is for no missing case, curve 2 is for (1 , 1) missing case, 3 is for (0 , 0) missing case, and 4 is for $(\alpha, 0)$ missing case. We can see in this figure that missing of an axial point has a bad effect on D-optimality, and this bad effect is serious as α becomes larger. But, it looks that the missing of center point or factorial point makes the design better in sense of D-optimality. This is due to the fact that the experimental point near center point has bad influence on D-optimality in every design. So D-optimality has tendency of excluding the points near center point, and of including the points far from center point. Therefore, as α becomes larger, the missing of axial point has worse influence on D-optimality.

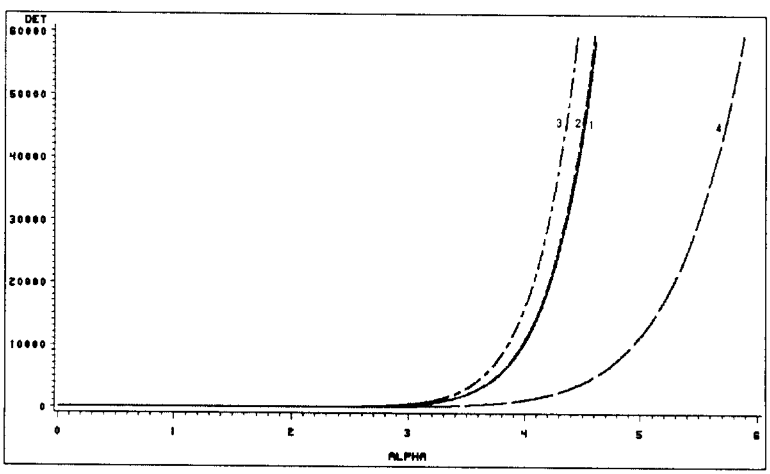

Figure 4-1. Determinant of moment matrix

To investigate more detail, see Figure 4-2 which is drawn with the ratio of determinant of moment matrix. Here, the ratio in the y-axis means the following value ;

$$RAT = \frac{|M| \text{ with missing cell}}{|M| \text{ without missing cell}}$$

Each curve in Figure 4-2 is a graph of ratio versus α. The numbered 1 curve is for the missing of center point, the numbered 2 is for the missing of factorial point, and the numbered 3 is for the missing of axial point. Note that the determinant ratio is near 0 when α is about 1.414 and the center point is missing. It means that the missing of center point has seriously bad influence on the determinant of moment matrix when α is about 1.414. The CCD with two variables and one center point has rotatability when α is $\sqrt{2}$. But in this case, D-optimality is badly affected by the missing of center point. Also, we can see that the missing of axial point has worse effect on the determinant of moment matrix as α becomes larger.

In the beginning of this section, we saw that large value of α is better in the sense of D-optimality. But, large α is bad if we had a missing observation on axial point. To avoid a damage which we may receive from a missing cell, small or very large value is not preferable in CCD

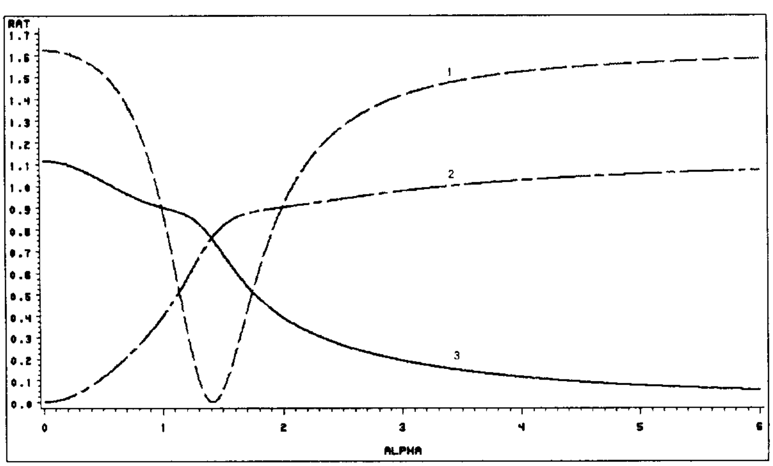

Figure 4-2. Ratio of determinant

4.3. A-Optimality

The concept of A-optimality deals with the individual variances of the regression coefficients. Unlike D-optimality, it does not make use of covariances among coefficients. Note that the variances of regression coefficients appear on the diagonals of $(X'X)^{-1}$. A-optimality is defined as

$$\min_{\zeta} \; tr(M(\zeta))^{-1}$$

where $M(\zeta)$ is the design moment for a particular design selection ζ, and tr represents trace, that is, the sum of the variances of the coefficients (weighted by N).

In Section 2, we discussed the variances of regression coefficients respectively. But in Section 4-4, in the sense of A-optimality, we will investigate the variances of regression coefficients together.

4.4. Influence of a missing cell on A-Optimality

Generally speaking, the trace of inverse of moment matrix decreases as the value of α increases. But, what happens if there is a missing cell ? In the previous section, we saw that the determinant of moment matrix increases as the value of α increases, whether there is a missing cell or not. However, the trace of inverse of moment matrix does not always decrease as α increases. Figure 4-3 shows four trace curves of CCD with two variables and one center point.

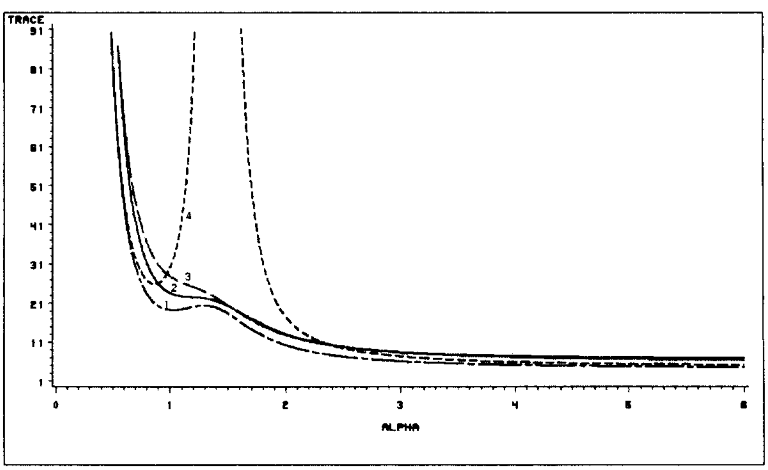

Figure 4-3. Trace of inverse of moment matrix

The numbered 1 curve shows the trace of inverse of moment matrix when there is no missing cell. It has an interval in which the value of trace increases as α increases. The curves 2 and 3 are the trace of inverse of moment matrix when there is a missing cell on an axial point and a factorial point, respectively. The value of trace always decreases as α increases. When the center point is missing, curve 4, the value of trace is extremely large if α lies on near 1.4. It means that the variances of certain coefficients are very large. We saw, in Section 4-2, that the same problems occur in D-optimality.

To investigate more detail, see Figure 4-4 which is drawn with the ratio of trace of inverse of moment matrix. Here, the ratio in the y-axis means the following value ;

$$RAT = \frac{tr(M^{-1}) \quad \text{with missing cell}}{tr(M^{-1}) \quad \text{without missing cell}}$$

In Figure 4-4, curve 1 is for missing of the center point, curve 2 is for missing of the factorial point, and curve 3 is for missing of the axial point. We can see in this figure that the missing of factorial point or axial point does not make serious problem in A-optimality, but the missing of center point can cause the worst A-optimality.

In conclusion, α larger than 2 makes the design better, whether there is a missing cell or not. We saw that APV is badly affected by missing on the center point when α is between 1 and 2. Here, the A-optimality is also seriously damaged in the same case.

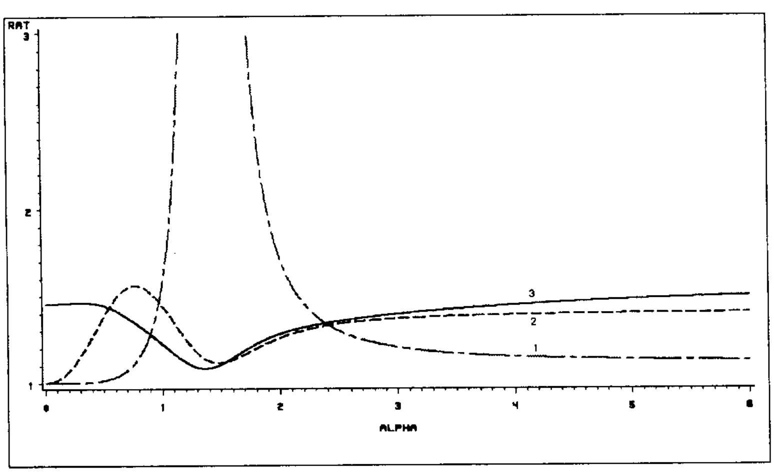

Figure 4-4. Ratio of trace

5. CONCLUDING REMARKS

Until now, we examined the influences of a missing cell in CCD. In this article, CCD with two variables and one center point is mainly discussed. CCD with more variables or center points can be examined in the same way.

The influences of missing cells on the center point, factorial point, and axial point are somewhat different. In any case, too small (less than 0.5) or large value (larger than 3) is not preferable for α. Especially, the missing on the center point must be carefully examined. When CCD with two variables and one center point is considered, the missing on the center point causes a serious problem on APV, D-optimality or A-optimality if α is near to $\sqrt{2}$. That is, we must be careful so that the missing on center point does not occur when we use the rotatable central composite design.

Myers, Khuri and Carter(1989) discussed about the choice of α and the number of center points. The choice of α depends on the experimenter. If we consider the cases discussed in this paper, we can choose α which makes the design better in the sense of robustness to a missing cell.

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