Journal of the KSQC
Vol. 19, No. 2, Dec.1991

1991년 12월 韓國品質管理學會誌 제19권 제2호

A Graphical Method for Evaluating the Effect of Outliers, Missing Observations, and Design Augmentation in the Slope Estimation of Response Surface Designs

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ABSTRACT

In many applications of response surface methodology, good estimation of the derivatives of the response function may be as important or perhaps more important than estimation of mean response. Using a graphical method, we have studied the effect of outliers, missing observations, and design augmentation with respect to the slope estimation in the response surface designs.

1. Introduction

In many application of response surface methodology, good estimation of the derivatives of the response function may be as important or perhaps more important than estimation of mean response. The partial derivatives are important when the rate of change of mean response with respect to any or all of the design variables is critical. Certainly, optimum seeking methods - the usual stationary point

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calculation in a second-order analysis, steepest ascent method and ridge analysis - depends heavily on the partial derivatives of the estimated response function with respect to the design variables. Since designs that attain certain properties in estimated response do not enjoy the same properties for the estimated slope, it is important for the user to consider experimental designs that are constructed with the derivatives. Therefore, recent work in the design of experiments for response surface analysis has focused attention on the estimation of partial derivatives of the response function with respect to the explanatory variables. Herzberg (1967), Atkinson (1970), Murty and Studden (1972), Ott and Mendenhall (1972), Myers and Lahoda (1975), Hader and Park (1978), Box and Draper (1980), Huda and Mukerjee (1984), Mukerjee and Huda (1985), Park (1987), Koske (1989), Park (1990) and others have considered problems associated with estimation of derivatives of the response function or of the difference between two responses.

A graphical metthod of assessing the prediction capability of response surface designs was introduced by Giovannitti-Jensen and Myers (1989). Vining and Myers (1991) developed a graphical approach for evaluating response surface designs in terms of the mean squared error of prediction. In this paper, using a similar graphical method, we have studied the effect of outliers, missing observations, and design augmentation with respect to the slope estimation in the response surface designs.

2. Spherical region moments

It is assumed that the response relationship is adequately approximated by the second-order polynomial model in k independent variable, $\underline{x}' = (x_1, x_2, \cdots, x_k)$.

$$\eta(\underline{x}) = \beta_0 + \sum_{i=1}^{k}\beta_i x_i + \sum_{i=1}^{k}\beta_{ii} x_i^2 + \sum_{\substack{i=1\\ i<j}}^{k}\sum_{j=1}^{k}\beta_{ij}\, x_i\, x_j, \tag{2.1}$$

which may be writtenn in matrix notation as

$$\eta(\underline{x}) = \underline{x}_s'\ \beta, \tag{2.2}$$

in which the $1 \times p$ vector $\underline{x}_s' = (1, x_1, x_2, \cdots, x_k, x_1^2, \cdots, x_k^2, x_1 x_2, \cdots, x_{k-1} x_k)$ and $\underline{\beta}$ is the $p \times 1$ column vector of the corresponding coefficents. Here $p = 2k + \binom{k}{2} + 1$ is the number of parameters in the model. As usual the design variables x's are transformations of the experimental variables. By the method of least squares, the fitted equation $y(\underline{x}) = \underline{x}_s'\ \underline{b}$ is to be used to estimate $\eta(\underline{x})$.

Let the estimated slope vector be denoted by

$$\underline{g}(\underline{x}) = \begin{pmatrix} \partial\hat{y}/\partial x_1 \\ \partial\hat{y}/\partial x_2 \\ \vdots \\ \partial\hat{y}/\partial x_k \end{pmatrix} = D\underline{b}, \tag{2.3}$$

where $D = [\underline{0}, I_k, 2\mathrm{diag}(x_1, \cdots, x_k), D^*]$ is the matrix arising from the differentiation of $\underline{x}_s{}'\underline{b}$ with respect to each of the k design variables. Here the matrix

$$D^* = \begin{pmatrix} x_2 & x_3 & \cdots & x_k & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ x_1 & 0 & \cdots & 0 & x_3 & x_4 & \cdots & x_k & \cdots & 0 & 0 & 0 \\ 0 & x_1 & \cdots & 0 & x_2 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & x_2 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & x_{k-1} & x_k & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & x_{k-2} & 0 & x_k \\ 0 & 0 & \cdots & x_1 & 0 & 0 & \cdots & x_2 & \cdots & 0 & x_{k-2} & x_{k-1} \end{pmatrix}$$

A spherical region moment of order δ is defined to be

$$\sigma_{\delta_1\delta_2\cdots\delta_k} = \psi \int_{U_r} x_1^{\delta_1} x_2^{\delta_2} \cdots x_k^{\delta_k}\, d\underline{x},$$

where $\psi^{-1} = \int_{U_r} d\underline{x} = 2\pi^{\frac{k}{2}}/\Gamma(\frac{k}{2})$ is the surface area of $U_r = \{\underline{x} : \sum_{i=1}^{k} x_i^2 = r^2\}$ and $\sum_{i=1}^{k}\delta_i = \delta$. If any δ_i is 0 that subscript is dropped from the designation of the moment. Since U_r is a symmetric region, the spherical moment $\sigma_{\delta_1\delta_2\cdots\delta_k}$ is 0 whenever any δ_i is odd.

The spherical region moments that are used in the second-order moder case are the second and fourth order spherical moments given by

$$\sigma_2 = \psi \int_{U_r} x_i^2\, d\underline{x} = \frac{r^2}{k},$$

$$\sigma_4 = \psi \int_{U_r} x_i^4\, d\underline{x} = \frac{3r^4}{k(k+2)}, \tag{2.4}$$

and

$$\sigma_{22} = \psi \int_{\mathcal{V}_r} x_i^2 x_j^2 \, dx = \frac{r^4}{k(k+2)}.$$

The above moments can be shown in terms of spherical coordinates. The spherical region moments do not depend in any way on the experimental design or form of the model used in the analysis. Region moments, as the name suggests, only depend on the region of interest. That is, they are functions of the radius r, and dimension k of the hypersphere under consideration.

Define the *spherical region moment matrix* S by

$$S = \psi \int_{\mathcal{V}} D' D dx \qquad (2.5)$$

3. The Effect of Outliers, Missing Observations, and Design Augmentation with respect to the Slope Estimation

3.1 Mean Shift Outlier Model

In response surface methodology, there is always a possibility that discordant observations will appear. In this section the only type of discordant observations to be addressed are these which result from inconsistency in the response variable. Those observations will be refered to as outliers.

The mean shift outlier model is defined by Cook and Weisberg (1982) as the following :

$$\underline{y} = X\underline{\beta} + \underline{d}_i\phi + \underline{\varepsilon}. \qquad (3.1)$$

where $\underline{d}_i$ is an index vector with a 1 in the i^{th} position and zeros elsewhere, and ϕ is the amount of the mean shift. Therefore, if ϕ is nonzero the i^{th} point is an outlier. The usual assumptions are made on $\underline{\varepsilon}$ and least squares estimation will be employed.

The outlier in this case induces bias into the squares estimator, $\underline{b}$, and thus into the estimated response, $\hat{\underline{y}}$ The biases are

$$\text{Bias}(\underline{b}) = (X'X)^{-1}\underline{x}_i\phi$$

$$\text{Bias}(\hat{\underline{y}}) = X(X'X)^{-1}\underline{x}_i\phi$$

where $\underline{x}_i' = (1, x_{1i}, x_{2i}, \cdots, x_{ki}, x_{1i}^2, x_{2i}^2, \cdots, x_{ki}^2, x_{1i}x_{2i}, \cdots, x_{k-1,i}x_{ki})$. The effect of tthe experimental design on the biases is seen by the role of $(X'X)^{-1}$.

To gain further insight into the effect of the outlier, consider the following matrix ;

$$H = X(X'X)^{-1}X'.$$

The elements of H will be denoted by h_{ij}.

$$h_{ij} = \underline{x}_i'(X'X)^{-1}\underline{x}_j = h_{ji} \qquad (3.2)$$

If $i = j$ then we have the diagonal elements of H. Hoaglin and Welsch (1978) refer to H as the hat matrix and diagonal elements of H as the hat diagonals.

3.2 Criteria of Outliers

Criteria will be developed for determining when the outlier is degrading. The criteria to be considered are as follows ;

1) Sum of the mean square errors of estimated slope vector $\hat{\underline{g}}(\underline{x})$

2) Sum of spherical mean square errors of estimated slope vector $\hat{\underline{g}}(\underline{x})$

Ⅰ. Sum of the Mean Square Errors of Estimated Slope Vector $\hat{\underline{g}}(\underline{x})$

In general the mean square error is defined as.

$$\text{MSE} = \text{Variance} + \text{Bias}^2.$$

From this define the mean square matrix for $\hat{\underline{g}}(\underline{x})$ to be

$$\text{MSE}(\hat{\underline{g}}(\underline{x})) = Var(\hat{\underline{g}}(\underline{x})) + \text{Bias}(\hat{\underline{g}}(\underline{x})) \cdot \text{Bias}(\hat{\underline{g}}(\underline{x}))'. \qquad (3.3)$$

The variance of $(\hat{\underline{g}}(\underline{x}))$ is

$$Var(\hat{\underline{g}}(\underline{x})) = Var(D\underline{b}) = D\,(X'X)^{-1}\,D'\sigma^2 \tag{3.4}$$

and the bias of $\hat{\underline{g}}(\underline{x})$ is

$$\text{Bias}(\hat{\underline{g}}(\underline{x})) = E(\hat{\underline{g}}(\underline{x})) - \underline{g}(\underline{x}) = E(D\underline{b}) - D\underline{\beta} = D(X'X)^{-1}\,\underline{x}_i\phi. \tag{3.5}$$

Therefore,

$$\text{MSE}(\hat{\underline{g}}(\underline{x})) = \sigma^2 D(X'X)^{-1}D' + \phi^2 D(X'X)^{-1}\underline{x}_i\underline{x}_i'(X'X)^{-1}D'.$$

An obvious norm to be used in developing a criteria is the sum of the mean square errors of $\hat{\underline{g}}(\underline{x})$, which is obtained from $\text{MSE}(\hat{\underline{g}}(\underline{x}))$ by taking the trace of the matrix. It can seen that

$$tr\,[\text{MSE}(\hat{\underline{g}}(\underline{x}))] = tr\,[\sigma^2 D\,(X'X)^{-1}\,D' + \phi^2 D(X'X)^{-1}\,\underline{x}_i\underline{x}_i'\,(X'X)^{-1}\,D']$$

$$= \sigma^2 tr\,[D'D(X'X)^{-1}] + \phi^2\underline{x}_i'(X'X)^{-1}\,D'D(X'X)^{-1}\,\underline{x}_i. \tag{3.6}$$

It is clear from (3.6) that the effect of the outlier on the sum of the mean squares errors of estimated slope vector is determined not only by the magnitude of the outlier but also by the location of the i^{th} point in the design space, as measured by $\underline{x}_i'(X'X)^{-1}\,D'D(X'X)^{-1}\,\underline{x}_i$, which is not scale free as the hat diagonal is.

The effects of eliminating the outlier, the i^{th} point, must also be considered. Let X_{-i} denote the matrix with the i^{th} row deleted, $\underline{y}_{-i}$ denote the response vector with the i^{th} observation deleted and $\underline{b}_{-i}$, and $\hat{\underline{g}}_{-i}(\underline{x})$ denote the least squares estimator and the estimated slope vector obtained with the i^{th} observation deleted respectively, i.e.,

$$\hat{\underline{g}}_{-i}(\underline{x}) = D\underline{b}_{-i}$$

where $\underline{b}_{-i} = (X_{-i}' X_{-i})^{-1} X_{-i}' \underline{y}_{-i}$.

Then as long as $N - 1 \geq p$ it is obvious that

$$E(\hat{\underline{g}}_{-i}(\underline{x})) = D\underline{\beta}$$

and

$$Var(\underline{g}_{-i}(\underline{x})) = \sigma^2 D(X_{-i}' X_{-i})^{-1} D'. \tag{3.7}$$

It can be shown that

$$(X_{-i}' X_{-i})^{-1} = (X' X)^{-1} + \frac{(X' X)^{-1}\underline{x}_i\underline{x}_i'(X' X)^{-1}}{1 - h_{ii}} \tag{3.8}$$

where h_{ii} is defined as in (3.2) (See Rao(1973), p. 33).

Since $\hat{\underline{g}}_{-i}(\underline{x})$ is unbiased for $D\underline{\beta}$, its mean square error matrix is simply its variance-covariance matrix. Then from (3.7) and (3.8)

$$\text{MSE}(\hat{\underline{g}}_{-i}(\underline{x})) = \sigma^2 D\,[(X' X)^{-1} + \frac{(X' X)^{-1}\underline{x}_i\underline{x}_i'(X' X)^{-1}}{1 - h_{ii}}]\,D'. \tag{3.9}$$

The mean square errors of the estimated slope vector wwith i^{th} observation deleted are found on the diagonal of the matrix given in (3.9). The sum of the mean square errors can then be found by taking the trace of the matrix as follows :

$$tr\,[\text{MSE}(\hat{\underline{g}}_{-i}(\underline{x}))] = \sigma^2 tr\,[D(X' X)^{-1} D' + \frac{D(X' X)^{-1}\underline{x}_i\underline{x}_i'(X' X)^{-1}D'}{1 - h_{ii}}]$$

$$= \sigma^2\,[tr[D' D(X' X)^{-1}] + \frac{\underline{x}_i'(X' X)^{-1}D' D(X' X)^{-1}\underline{x}_i}{1 - h_{ii}}]. \tag{3.10}$$

It can be seen from the relationship (3.10) that $\underline{x}_i'(X'X)^{-1}D'D(X'X)^{-1}\underline{x}_i$ not only plays a role in determining the effect of the outlier, but also in determining the effect of deleting the observation.

Recall that it is desirable to choose the estimator which is more accurate, in this case either $\underline{b}$ or $\underline{b}_{-i}$. If $\underline{b}_{-i}$ is more accurate than $\underline{b}$, this indicates that the outlier is causing undue harm and should be discarded. Thus, if the sum of the mean square errors for $\hat{\underline{g}}(\underline{x})$ is larger than the sum of the mean square errors for $\hat{\underline{g}}_{-i}(\underline{x})$, the outlier is degrading the analysis. The following theorem provides the condition under which inclusion of the point is degrading to the analysis.

Theorem 3.1 $tr[\text{MSE}(\hat{\underline{g}}(\underline{x}))] > tr[\text{MSE}(\hat{\underline{g}}_{-i}(\underline{x}))]$ iff $\frac{\phi^2}{\sigma^2} > \frac{1}{1-h_{ii}}$.

Proof. $tr[\text{MSE}(\hat{\underline{g}}(\underline{x}))] > tr[\text{MSE}(\hat{\underline{g}}_{-i}(\underline{x}))]$

$$\Leftrightarrow \sigma^2 tr[D'D(X'X)^{-1}] + \phi^2 \underline{x}_i'(X'X)^{-1}D'D(X'X)^{-1}\underline{x}_i$$

$$> \sigma^2 \left[tr[D'D(X'X)^{-1}] + \frac{\underline{x}_i'(X'X)^{-1}D'D(X'X)^{-1}\underline{x}_i}{1-h_{ii}} \right]$$

$$\Leftrightarrow \phi^2 \underline{x}_i'(X'X)^{-1}D'D(X'X)^{-1}\underline{x}_i > \sigma^2 \quad \frac{\underline{x}_i(X'X)^{-1}D'D(X'X)^{-1}\underline{x}_i}{1-h_{ij}}$$

$$\Leftrightarrow \phi^2 > \frac{\sigma^2}{1-h_{ii}}$$

$$\Leftrightarrow \frac{\phi^2}{\sigma^2} > \frac{1}{1-h_{ii}}.$$

If the relationship stated in Theorem 3.1 holds, then the outlying observation should be discarded.

Ⅱ. Sum of Spherical Mean Square Errors of Estimated Slope Vector $\hat{\underline{g}}(\underline{x})$

If the experimenter is interested in predicting the response slope throughout the surface of a hypersphere, then a appropriate criteria is the spherical mean square error of estimated slope vector.

Spherical mean square error of $\hat{\underline{g}}(\underline{x})$ is defined to be

$$\mathrm{SMSE}(\hat{\underline{g}}(\underline{x})) = \frac{N\psi}{\sigma^2}\int_{U_r}\mathrm{MSE}(\hat{\underline{g}}(\underline{x}))\,d\underline{x}$$

$$= \frac{N\psi}{\sigma^2}\int_{U_r}Var(\hat{\underline{g}}(\underline{x}))\,d\underline{x} + \frac{N\psi}{\sigma^2}\int_{U_r}\mathrm{Bias}^2(\hat{\underline{g}}(\underline{x}))\,d\underline{x} \qquad (3.11)$$

where $\underline{U}_r = \{\underline{x}: \sum_{i=1}^{k} x_i^2 = r^2\}$ and $\psi^{-1} = \int_{U_r} d\underline{x}$.

The first term in (3.11), is given as

$$SV(\hat{\underline{g}}(\underline{x})) = \frac{N\psi}{\sigma^2}\int_{U_r}Var(\hat{\underline{g}}(\underline{x}))\,d\underline{x}$$

$$= \frac{N\psi}{\sigma^2}\int_{U_r}E[\hat{\underline{g}}(\underline{x}) - E(\hat{\underline{g}}(\underline{x}))]'[\hat{\underline{g}}(\underline{x}) - E(\hat{\underline{g}}(\underline{x}))]\,d\underline{x}$$

$$= \frac{N\psi}{\sigma^2}\int_{U_r}E[(\underline{b} - E(\underline{b}))'\,D'D\,(\underline{b} - E(\underline{b}))]\,d\underline{x}$$

$$= \frac{N\psi}{\sigma^2}\int_{U_r}tr\,\{D'DE[(\underline{b} - E(\underline{b}))\,[b - E(b))']\}\,d\underline{x}$$

$$= Ntr\,(S\,(X'X)^{-1}). \qquad (3.12)$$

The the second term in (3.11), is given as

$$SB(\hat{\underline{g}}(\underline{x})) = \frac{N\psi}{\sigma^2}\int_{U_r}\mathrm{Bias}^2\,(\hat{\underline{g}}(\underline{x}))\,d\underline{x}$$

$$= \frac{N\psi}{\sigma^2}tr\int_{U_r}[E\,(\hat{\underline{g}}(\underline{x})) - \underline{g}(\underline{x})]'[E(\hat{\underline{g}}(\underline{x})) - \underline{g}(\underline{x})]\,d\underline{x}$$

$$= \frac{N\psi\phi^2}{\sigma^2} \int_{U_r} \underline{x}_i' \ (X'X)^{-1} D'D (X'X)^{-1} \ \underline{x}_i \, d\underline{x}$$

$$= \frac{N\phi^2}{\sigma^2} [\underline{x}_i' \ (X'X)^{-1} S (X'X)^{-1} \ \underline{x}_i]. \tag{3.13}$$

From (3.12) and (3.13),

$$\text{SMSE}(\hat{\underline{g}}(\underline{x})) = Ntr[S(X'X)^{-1}] + \frac{N\phi^2}{\sigma^2}[\underline{x}_i'(X'X)^{-1} S (X'X)^{-1} \underline{x}_i]. \tag{3.14}$$

To determine the effect of deleting the outlying observation, let X_{-i}, $\underline{y}_{-i}$ and $\underline{b}_{-i}$ be as previously defined. From (3.7) and (3.8),

$$\text{SMSE}(\hat{\underline{g}}_{-i}(\underline{x})) = \frac{N\psi}{\sigma^2} \int_{U_r} Var(\hat{\underline{g}}_{-i}(\underline{x}))\, dx$$

$$= \frac{N\psi}{\sigma^2} \int_{U_r} E[\hat{\underline{g}}_{-i}(\underline{x}) - E(\hat{\underline{g}}_{-i}(\underline{x}))]'[\hat{\underline{g}}_{-i}(\underline{x}) - E(\hat{\underline{g}}_{-i}(\underline{x}))]\, d\underline{x}$$

$$= \frac{N\psi}{\sigma^2} \int_{U_r} E[\underline{b}_{-i} - E(\underline{b}_{-i}))' D'D (\underline{b}_{-i} - E(\underline{b}_{-i}))]\, d\underline{x}$$

$$= \frac{N\psi}{\sigma^2} \int_{U_r} tr\{D'DE[(\underline{b}_{-i} - E(\underline{b}_{-i}))\ [\underline{b}_{-i} - E(\underline{b}_{-i}))']\}\, d\underline{x}$$

$$= Ntr[\ S(X'X)^{-1} + \frac{(X'X)^{-1}\underline{x}_i\underline{x}_i'\ (X'X)^{-1}}{1 - h_{ii}}]$$

$$= Ntr[\ S(X'X)^{-1}\ ] + \frac{N}{1-h_{ii}}[\ \underline{x}_i'(X'X)^{-1} S (X'X)^{-1}\ \underline{x}_i]. \tag{3.15}$$

Now, the two spherical mean square errors must be compared to determine under what condition the outlier is deteriorating the analysis. This condition is given by the following theorem.

Theorem 3.2 $\text{SMSE}(\hat{\underline{g}}(\underline{x})) > \text{SMSE}(\hat{\underline{g}}_{-i}(\underline{x}))$ iff $\frac{\phi^2}{\sigma^2} > \frac{1}{1-h_{ii}}$.

Proof. $\text{SMSE}(\hat{g}(\underline{x})) > \text{SMSE}(\hat{g}_{-i}(\underline{x}))$

$$\Leftrightarrow N tr[S(X'X)^{-1}] + \frac{N\phi^2}{\sigma^2}[\underline{x}_i'(X'X)^{-1}S(X'X)^{-1}\underline{x}_i]$$

$$> N tr[S(X'X)^{-1}] + \frac{N}{1-h_{ii}}[\underline{x}_i'(X'X)^{-1}S(X'X)^{-1}\underline{x}_i]$$

$$\Leftrightarrow \frac{N\phi^2}{\sigma^2}[\underline{x}_i'(X'X)^{-1}S(X'X)^{-1}\underline{x}_i]$$

$$> \frac{N}{1-h_{ii}}[\underline{x}_i'(X'X)^{-1}S(X'X)^{-1}\underline{x}_i]$$

$$\Leftrightarrow \frac{\phi^2}{\sigma^2} > \frac{1}{1-h_{ii}}. \quad ¶$$

Thus, all of the criteria considered, yield the same result. The experimenter in practice will not know whether or not the condition holds. Hence, we can test the null hypothesis that

$$H_0 : \frac{\phi^2}{\sigma^2} \leq \frac{1}{1-h_{ii}} \quad H_1 : \frac{\phi^2}{\sigma^2} > \frac{1}{1-h_{ii}}$$

The following theorem (See O'Gorman (1984)) gives the distribution of the statistic.

Theorem 3.3 Under the mean shift outlier model given in (3.1) with the usual least squares assumptions on $\underline{\varepsilon}$ and with the additional assumption that each term in the $\underline{\varepsilon}$ vector has a normal distribution, then

$$(RSTUDENT_i)^2 = \frac{\hat{\varepsilon}_i^2}{s_{-i}^2(1-h_{ii})} \sim F'_{1,\,N-P-1,\,\lambda},$$

where $\lambda = \frac{\phi^2(1-h_{ii})}{2\sigma^2}$ is non-centrality parameter, $\hat{\underline{\varepsilon}}_i$ is the residual at the i^{th} point and s_{-i}^2 is the residual mean square computed without the i^{th} point.

Hence, we reject H_0 if $(RSTUDENT_i)^2$ is greater than or equal to the $(1-\alpha)$ percentage point for the noncentral F distribution with degree of freedom 1 and $N-p-1$ and non-centrality parameter $\lambda = \frac{1}{2}$.

3.3 The Effect of Outliers

Let us assume that a single outlier may occur at any one of the design points. The mean shift outlier model given in (3.1) will be used in representing the occurrence of an outlier. Under this model the estimated slope vector at an arbitrary point in the design space is biased.

Let B_i denote the sum of the squared biases in the estimated slope vector $\hat{\underline{g}}(\underline{x})$ due to an outlier at the i^{th} design point. Without loss of generality, we assume $\phi^2 = 1$. Then, from (3.6)

$$B_i = \underline{x}_i'(X'X)^{-1} D'D(X'X)^{-1}\underline{x}_i.$$

Let $\bar{B}_i(r)$ denote the spherical squared bias in the estimated slope vector $\hat{\underline{g}}(\underline{x})$ due to an outlier at the i^{th} design point (apart from $\frac{N\phi^2}{\sigma^2}$). Then, from (3.14)

$$\bar{B}_i(r) = \underline{x}_i'(X'X)^{-1} S(X'X)^{-1} \underline{x}_i.$$

We can plot $\bar{B}_i(r)$ with a measure that depicts the lack of stability of $\bar{B}_i(r)$ as a deviation from the average given by $\bar{B}_i(r)$. We define the range of B_i on the sphere of radius r as

$$RB_i(r) = \max_{\underline{x}\in U_r} B_i - \min_{\underline{x}\in U_r} B_i.$$

We will use $RB_i(r)$ as the dispersion measure depicted graphically. For a given design there will then be N possible $\bar{B}_i(r)$'s and $R\bar{B}_i(r)$'s, one for each of the points at which the outlier could occur.

Since the experimenter does not know a priori where the outlier will occur, he would like to choose a design which limits the effect of the outlier no matter where it occurs. This can be achieved by a minimax approach that minimizes over designs $Bout(r) = \max_i \max_{\underline{x}\in U_r} B_i$ with respect to r. Thus, the robust design is obtained by $\min_{D} Bout(r)$ with respect to r.

Example : Figure 3.1, Figure 3.2 and Figure 3.3 show $\bar{B}_i(r)$, $\max_{x \in U_r} B_i$ and $\min_{x \in U_r} B_i$, in the case that outliers are factorial point, axial point, and center point, respectively. By Figure 3.4, we can obtain the fact that experimenter must give attention to the outlier possibility of factorial point in the region $r \leq 0.4$ and center point in the region $r > 0.4$.

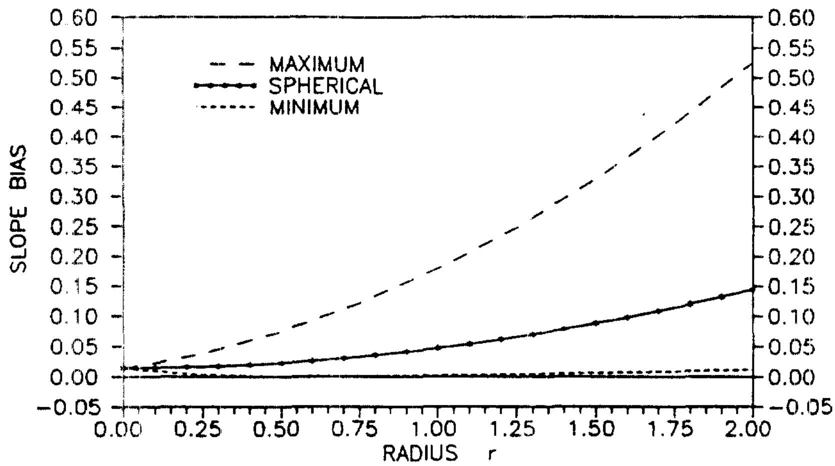

Figure 3.1. SPHERICAL SLOPE BIAS, MAXIMUM AND MINIMUM SLOPE BIASES DUE TO AN OUTLIER AT FACTORIAL POINTS OF CCD(α=1.682)

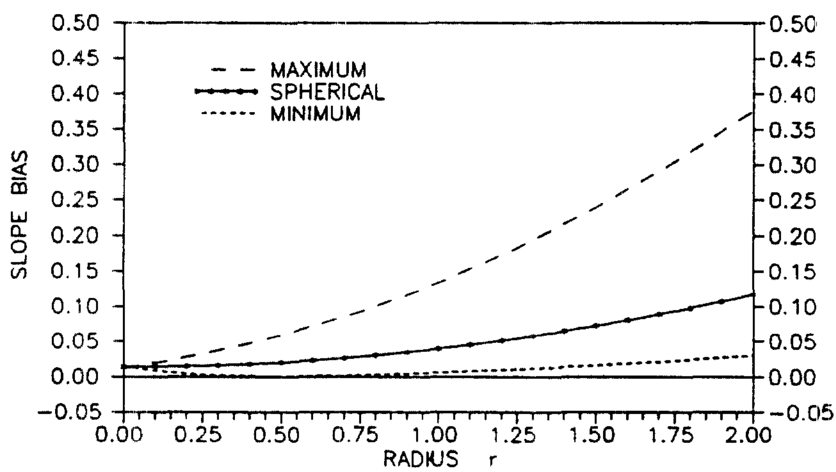

Figure 3.2. SPHERICAL SLOPE BIAS, MAXIMUM AND MINIMUM SLOPE BIASES DUE TO AN OUTLIER AT AXIAL POINTS OF CCD(α=1.682)

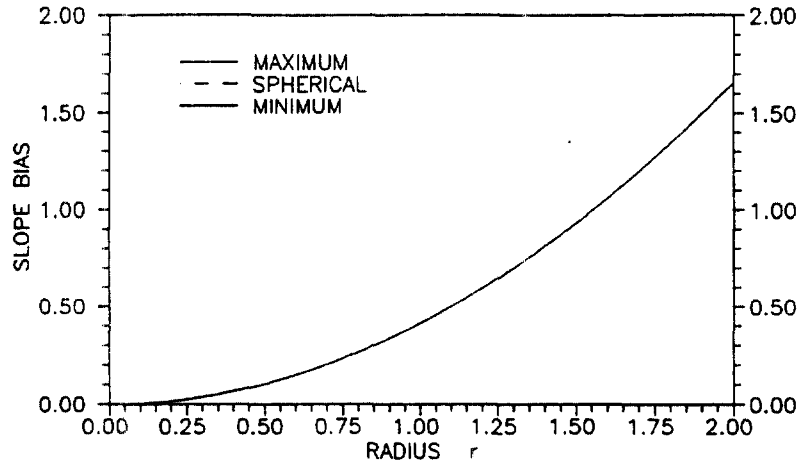

Figure 3.3. SPHERICAL SLOPE BIAS, MAXIMUM AND MINIMUM SLOPE BIASES DUE TO AN OUTLIER AT CENTER POINT OF CCD(α=1.682)

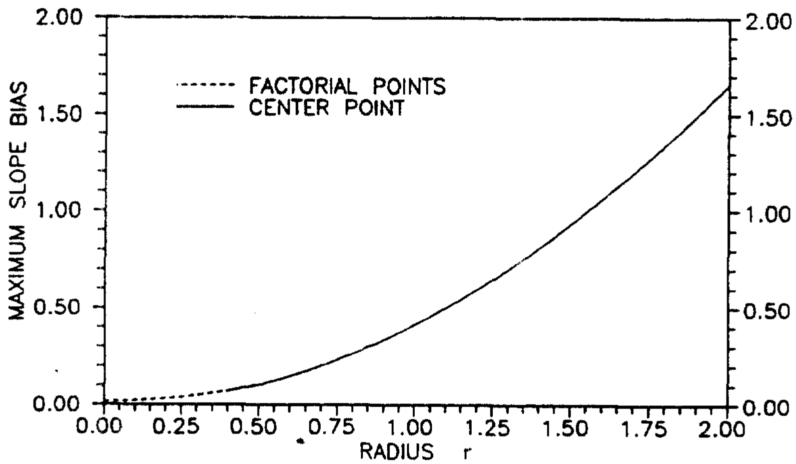

Figure 3.4. MAXIMUM SLOPE BIAS $B_{OUT}(r)$ OF CCD(α=1.682)

3.4 The Effect of Missing Observations

As seen in Section 3.1, when data is dropped from the analysis for some reason, it causes the variance of the estimated slope vector to become inflated. In this case the effects of losing a single data point will be investigated.

In (3.9) it is seen that the variance-covariance matrix of $\hat{\underline{g}}_{-i}(\underline{x})$ is

$$Var(\hat{\underline{g}}_{-i}(\underline{x})) = \sigma^2 D[(X'X)^{-1} + \frac{(X'X)^{-1}\underline{x}_i\underline{x}_i'(X'X)^{-1}}{1-h_{ii}}]D'.$$

Let

$$V_{-i} = \frac{tr[Var(\hat{g}_{-i}(\underline{x}))]}{\sigma^2}$$

$$tr[D'D(X'X)^{-1}] + \frac{1}{1-h_{ii}}\underline{x}_i'(X'X)^{-1}D'D(X'X)^{-1}\underline{x}_i$$

and

$$\bar{V}_{-i}(r) = \frac{\psi}{\sigma^2}\int_{U_r} tr[Var(\hat{\underline{g}}_{-i}(\underline{x}))]dx$$

$$= tr[S(X'X)^{-1}] + \frac{1}{1-h_{ii}}\underline{x}_i'(X'X)^{-1}S(X'X)^{-1}\underline{x}_i.$$

Then, we can plot $\bar{V}_{-i}(r)$ with measure that depicts the lack of stability of $\bar{V}_{-i}(r)$ as a deviation from the average given by $\bar{V}_{-i}(r)$. We define the range of V_{-i} on the sphere of radius r as

$$RV_{-i}(r) = \max_{x\in U_r} V_{-i} - \min_{x\in U_r} V_{-i}.$$

We will use $RV_{-i}(r)$ as the dispersion measure depicted graphically. For a given design there will then be N possible $\bar{V}_{-i}(r)$'s and $RV_{-i}(r)$'s, one each point in the design.

It will not be known proir to expermentation which point will be lost during the course of the experiment. So the experimenter should choose a design in this case which will result in the analysis being minimally affected if a point is lost, no matter which point in the design it might be. This can be achieved by a minimax approach that minimizes over designs $V_{miss}(r) = \max_i \max_{\underline{x}\in U_r} V_{-i}$ with respect to r. Thus, the robust design is obtained by $\min_D V_{miss}(r)$ with respect to r.

Example : Figure 3.5 and Figure 3.6 show $\bar{V}_{-i}(r)$, $\max_{\underline{x}\in U_r} V_{-i}$, and $\min_{\underline{x}\in U_r} V_{-i}$, in the case that missing observations are $(0, 0 \pm \sqrt{6})$ type and $(\pm 0.7507, \pm 2.1063, \pm 1)$ type of Roquemore 311B design, respectively. Because Roquemore 311B design requires center point to avoid singularity of the moment matrix, we must avoid to miss center point. By Figure 3.7, we can obtain the fact that experimenter must give attention to considerable slope variance increase due to a missing observation of (± 0.7507, ±2.1063, ±1) type.

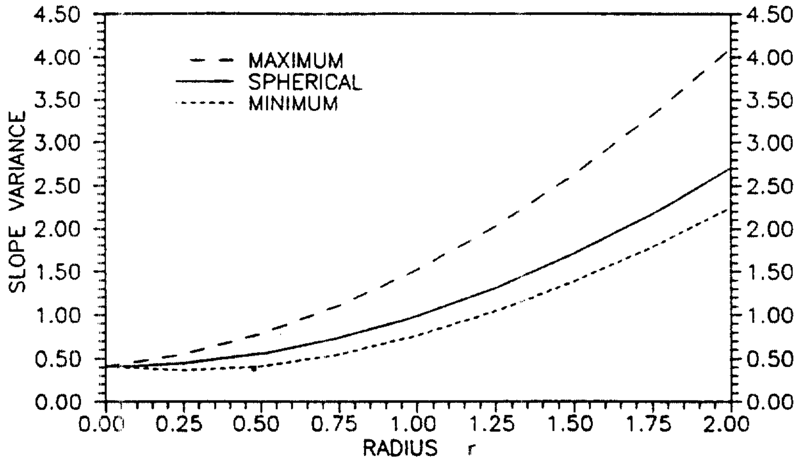

Figure 3.5. SPHERICAL SLOPE VARIANCE, MAXIMUM AND MINIMUM SLOPE VARIANCES DUE TO A MISSING OBSERVATION AT 1st OR 2nd POINT((0,0,$\pm\sqrt{6}$) TYPE) OF ROQUEMORE 311B DESIGN

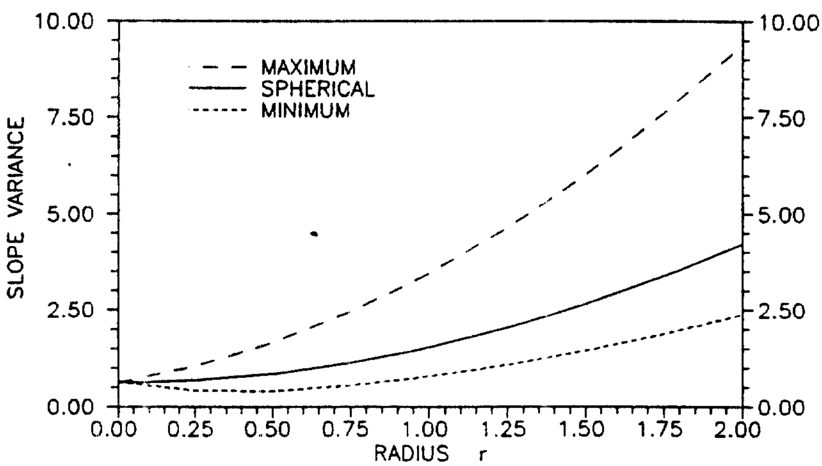

Figure 3.6. SPHERICAL SLOPE VARIANCE, MAXIMUM AND MINIMUM SLOPE VARIANCES DUE TO A MISSING OBSERVATION AT ANY ONE AMONG 3rd – 10th POINTS((±0.7507,±2.1063,±1) OR (±2.1063,±0.7507,±1) TYPE) OF ROQUEMORE 311B DESIGN

It is important to supplement the plot of $\bar{V}(r)$ of the equation (3.17) with some measure that depicts the lack of stability of the average slope variance function as a deviation from the average given by $\bar{V}(r)$. One needs to capture in a graphical way a sense of the distribution of $\bar{V}(\underline{x})/\sigma^2$ as function of r. Consider a measure of the variability in $\bar{V}(\underline{x})/\sigma^2$ where $\underline{x}$ takes values in U_r. We define the slope variance dispersion(SVD) measure, the range of $\bar{V}(\underline{x})/\sigma^2$ on the sphere of radius r, as

$$RV(r) = V\max(r) - V\min(r)$$

where $V\max(r) = \max_{\underline{x} \in U_r} \frac{\bar{V}(\underline{x})}{\sigma^2}$ and $V\min(r) = \min_{\underline{x} \in U_r} \frac{\bar{V}(\underline{x})}{\sigma^2}$.

With a view to improving the precision of the estimated slope vector, one might consider augmenting a point to the design in order to make the resulting spherical average slope variance on some sphere as small as possible. It is thought that the greatest improvemennt in the spherical average slope variances across all spheres would result from the minimization of the spherical average slope variance on the sphere corresponding to the largest $\bar{V}(r)$ for the original design. The minimization of the spherical average slope variance is conditional on the settings of the original design.

Consider a design with N design points to fit a model in k variables. Let $\underline{x}_a$ denote the point which is to be added to the design. The model-matrix corresponding to the design augmenting by $\underline{x}_a$ is then,

$$X_a = \binom{X}{\underline{x}_a'}$$

where $\underline{x}_a'$ has the same form as $\underline{x}_s$ in (2.2).

Letting $\bar{V}_a(\underline{x})$ represent the average slope variance obtained with the augmented design,

$$\frac{\bar{V}_a(\underline{x})}{\sigma^2} = \frac{1}{k} tr\left[D(X_a' X_a)^{-1} D'\right]$$

$$= \frac{1}{k} tr [D (X'X + \underline{x}_a \underline{x}_a')^{-1} D'].$$

The inverse, $(X'X + \underline{x}_a\underline{x}_a')^{-1}$, is found by applying the Sherman-Morrison-Woodbury theorem (Rao (1973) p. 33). Thus,

$$(X'X + \underline{x}_a\underline{x}_a')^{-1} = (X'X)^{-1} - \frac{(X'X)^{-1}\underline{x}_a\underline{x}_a'(X'X)^{-1}}{1+\underline{x}_a'(X'X)^{-1}\underline{x}_a}.$$

Then,

$$\frac{\overline{V}_a(\underline{x})}{\sigma^2} = \frac{1}{k} tr [D(X'X)^{-1}D'] - \frac{1}{k} tr \left[\frac{D(X'X)^{-1}\underline{x}_a\underline{x}_a'(X'X)^{-1}D'}{1+\underline{x}_a'(X'X)^{-1}\underline{x}_a} \right]$$

$$= \frac{1}{k} tr [D(X'X)^{-1}D'] - \frac{1}{k} \frac{\underline{x}_a'(X'X)^{-1}D'D(X'X)^{-1}\underline{x}_a'}{1+\underline{x}_a'(X'X)^{-1}\underline{x}_a}.$$

Therefore, the spherical average slope variance obtained with the augmented design is

$$\overline{V}_a(r) = \frac{1}{k} tr [S(X'X)^{-1}] - \frac{1}{k} \frac{\underline{x}_a'(X'X)^{-1}S(X'X)^{-1}\underline{x}_a}{1+\underline{x}_a'(X'X)^{-1}\underline{x}_a}$$

$$= \overline{V}(r) - \frac{1}{k} \frac{\underline{x}_a'(X'X)^{-1}S(X'X)^{-1}\underline{x}_a}{1+\underline{x}_a'(X'X)^{-1}\underline{x}_a}. \quad (3.18)$$

where the matrix S is the matrix of spherical moments defined by (2.5) for the model.

The suggested criterion requires the point $\underline{x}_a$ be chosen so that $\overline{V}_a(r)$ is minimized. Since the second term of the right hand side of (3.18) is nonnegative, this is equivalent to choosing $\underline{x}_a$ to maximize the quantity

$$\frac{\underline{x}_a'(X'X)^{-1}S(X'X)^{-1}\underline{x}_a}{1+\underline{x}_a'(X'X)^{-1}\underline{x}_a}.$$

To a researcher interest in predicting the slope of the response of a system, particularly on spheres, the spherical slope variance criteron may be more appealing than the conditional $|X'X|$ criterion.

Example. By Figure 3.8 we can know that the spherical average slope variance decrease due to design augmentation in CCD. But when we consider sample size, the spherical average slope variance decreases due to center point augmentation only in Figure 3.9.

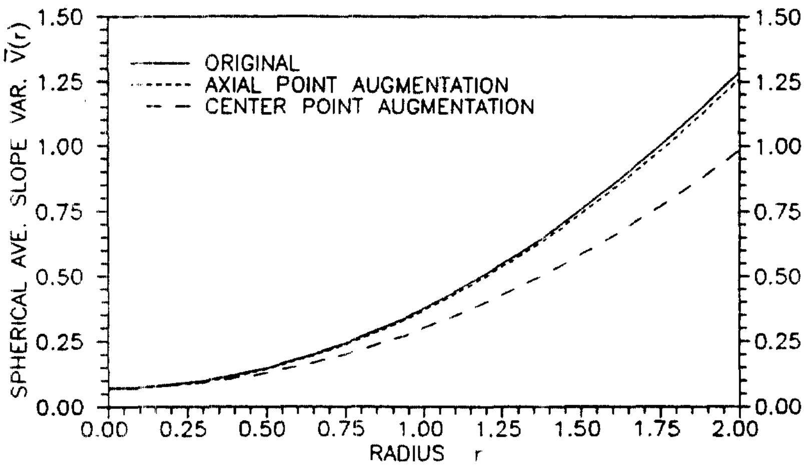

Figure 3.8. THE CHANGE OF SPHERICAL AVERAGE SLOPE VARIANCE $\bar{V}(r)$ DUE TO DESIGN AUGMENTATION IN CCD(α=1.682)

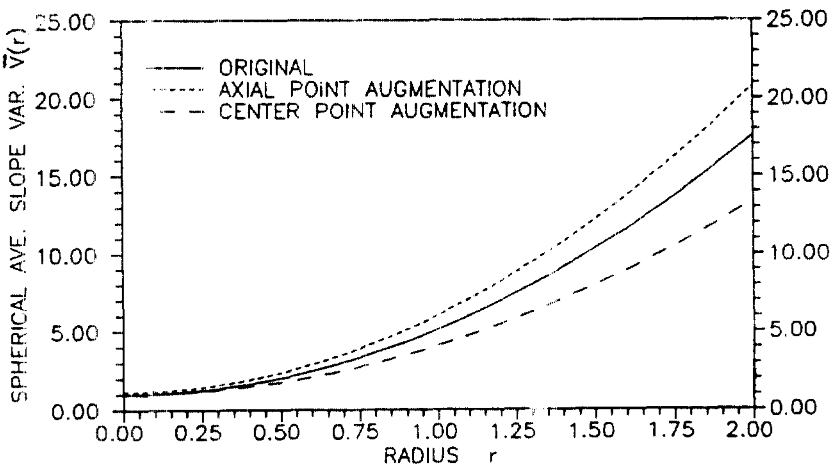

Figure 3.9. THE CHANGE OF SPHERICAL AVERAGE SLOPE VARIANCE $\bar{V}(r)$ DUE TO DESIGN AUGMENTATION IN CCD(α=1.682) (WEIGHTED BY SAMPLE SIZE)

4. Concluding Remarks

A graphical tool has been developed to measure the effect of outliers, missing observations, and design augmentation with respect to the slope estimation. The further study could be done to develop a graphical tool to measure the effect of outilers, missing observations, and design augmentation with respect to the estimation of prediction. By this graphical tool, response surface designs can be evaluated.

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