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Robust Designs to Outliers for Response Surface Experiments

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ABSTRACT

This paper treats a robust design criterion which minimizes the effects of outliers and model inadequacy, and investigates robust designs for some response surface designs. In order to develop a robust design criterion and robust design, the integrated mean squared error of $\hat{y}_m$ over a region is utilized, where $\hat{y}_m$ is the estimated response by the minimum bias estimation proposed by Karson, Manson and Hader (1969). According to the number of aberrant observations and their positions, the proposed criterion and designs are studied. Also further development of the proposed criterion is treated when outliers can occur in any position of a design.

1. Introduction

This paper considers a problem arising in the design of experiments for empirically investigating functional relationships between a dependent response variable and one or more independent continuous variables. Suppose that an experimenter wishes to explore a *functional relationship* between a response and several independent variables, $x_1, x_2, \cdots, x_p$, over some region R of experimental interest in the space of the quantitative factors.

The relationship could be expressed generally as

$$\eta(\underline{x})=f(\underline{x}, \underline{\beta}), \tag{1.1}$$

and observations $y_i(\underline{x})=\eta(\underline{x})+\varepsilon_i$ where $\underline{x}'=(x_1, x_2, \cdots, x_p)$, $\underline{\beta}'=(\beta_1, \beta_2, \cdots, \beta_r)$, and β_i's are unknown regression parameters which must be estimated by experimental data and assume that $\varepsilon_i \stackrel{iid}{\sim} (0, \sigma^2)$. If the true functional form $\eta(\underline{x})=f(\underline{x}, \underline{\beta})$ is unknown, as is often the case, the relationship may be approximated by the low order terms in the Taylor series expansion of the equation (1.1), which may be expressed as

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$$\eta(\underline{x}) = \beta_0 + \sum_{i=1}^{p} \beta_i x_i + \sum_{i\leq j=1}^{p} \beta_{ij} x_i x_j + \sum_{i\leq j\leq k=1}^{p} \beta_{ijk} x_i x_j x_k + \cdots. \tag{1.2}$$

The study of design optimality criteria has been of fundamental interest to researchers in the area of response surface analysis. Initially, criteria were largely concerned with variance, either of the individual coefficients or the fitted polynomial as a whole. In later work, the question of bias due to inadequacy of the approximating polynomial was considered by Box and Draper (1959). They proposed the minimization of the integrated mean squared error (*IMSE*) of $\hat{y}(\underline{x})$ over R (R is some region of the factor space of interest to the experimrnter.) as a basic criterion. This criterion considered bias and variance simultaneously. In general, the fitted equation $\hat{y}(\underline{x})$ in response surface experiments is intended to be used not only at the design points but with some region R. For enlightening references of response surface experiments for the use of some region of interest, the reader may refer of Myers(1976), Park(1977, 1978, 1981), Khuri and Cornell(1987) and Box and Draper(1987).

When model inadequacy exists, the *IMSE of* $\hat{y}(\underline{x})$ over R is

$$IMSE[\hat{y}] = V[\hat{y}] + B[\hat{y}], \tag{1.3}$$

where $V[\hat{y}] = \int_R Var[\hat{y}(\underline{x})]dW(\underline{x})$ is the integrated variance, and $B[\hat{y}] = \int_R \{E[\hat{y}(\underline{x})] - \eta(\underline{x})\}^2 dW(\underline{x})$ is the integrated squared bias, where $W(\underline{x})$ is a weighting probability distribution function on R.

In order to obtain $\hat{y}(\underline{x})$ the regression coefficients should be estimated from experimental data. Since the IMSE criterion was introduced, several authors have suggested different estimators for the regression coefficients to achieve smaller IMSE over R under some circumstances. In particular, Karson, Manson and Hader(1969) suggested the minimum bias estimator as an alternative to the least squares estimator for polynomial fits. If an estimable condition is satisfied, they show that the minimum bias estimator minimizes the integrated variance subject to the minimum integrated squared bias for any fixed design.

This paper considers design aspects of response surface experiments in which emphasis is on robust design to wild or "aberrant" observations. Based on designs in the space of the independent variables, the β_i's are estimated by the minimum bias estimation (*MBE*). In this paper, suppose an "aberrant" vector $\underline{d}' = (d_1, d_2, \cdots, d_n)$ is added to the observation vector $\underline{y}' = (y_1, y_2, \cdots, y_n)$, so that any i^{th} real observation $y_i + d_i$ can be an outlier. The $IMSE[\hat{y}_m]$ is used as a criterion on the accuracy of $\hat{y}_m(\underline{x})$, where $\hat{y}_m(\underline{x})$ is predicted value which is estimated by the *MBE*.

The main contents of this paper are to find a robust design criterion to some possible positions of outliers and to find robust designs, which are called R-designs will be found for the linear model when the true model is quadratic and for the quadratic model when the true model is cubic.

2. Development Of A Robust Design Criterion And Some Robust Designs

2.1 The Case of MBE

Most authors in describing optimal designs have used the estimation procedure of least squares.

When we are interested in bias caused by model inadequacy, it is natural to consider minimum bias. Minimization of this potential bias can be done by choice of design. The well-known estimation method is the *MBE* suggested by Karson, Manson and Hader(1969). An alternative strategy is to adopt a method of estimation aimed directly at minimizing bias and to use additional flexibility, if any, to satisfy other criteria.

Suppose the true model in (1.2) is a polynomial of degree c_2,

$$\eta(\underline{x})=\underline{x}_1'\beta_1+\underline{x}_2'\beta_2,$$

but the experimenter fits a polynomial of degree $c_1<c_2$, the first part $\underline{x}_1'\beta_1$. By the following lemma, we can obtain the $IMSE[\hat{y}_m]$ when the *MBE* is used, $\underline{d}$ exists and $\hat{y}_m$ is the fitted equation by MBE. Throughout this paper we will define the k_i's as follows :

$$k_i=\begin{cases} 1 \text{ if "aberrant" } d_i \text{ appears at the } i^{th} \text{ observation} \\ 0 \text{ otherwise.} \end{cases} \tag{2.1}$$

The matrix $K=diag(k_i)$ indicates the position of occurring "aberration".

Lemma 2.1

When $\eta(\underline{x})$ is estimated by $\hat{y}_m(\underline{x})=\underline{x}_1'\underline{b}_m$ ($\underline{b}_m=B\underline{b}$ is the minimum bias estimator of $\underline{\beta}_1$.) and aberrant vactor $\underline{d}$ exist, the *IMSE* of $\hat{y}_m(\underline{x})$ over the region R is expressed as follows :

$$IMSE[\hat{y}_m]=\sigma^2 Tr[B(X'X)^{-}B'M_{11}]+\underline{\beta}_2'P^*\underline{\beta}_2+\underline{d}'KS^*K\underline{d}, \tag{2.2}$$

where $B=(I\mid M_{11}^{-1}M_{12})$ and $\underline{b}=(X'X)^{-}X'\underline{y}$, Tr represents the trace, $P^*=M_{22}-M_{12}'M_{11}^{-1}M_{12}$, $S^*=T'B'M_{11}BT$ with $T=(X'X)^{-}X'$ and $M_{ij}=\int_R \underline{x}_i\underline{x}_j' dW(\underline{x})$.

proof

First, we have to obtain the $MSE[\hat{y}_m(\underline{x})]$. It can be readily shown that variance part and the bias part as follows :

$Var[\hat{y}_m(\underline{x})]=\underline{x}_1'B(X'X)^{-}B'\underline{x}_1\sigma^2$, and $Bias^2[\hat{y}_m(\underline{x})]=\{E[\hat{y}_m(\underline{x})]-\eta(\underline{x})\}^2=\underline{\beta}_2'(\underline{x}_1'M_{11}^{-1}M_{12}-\underline{x}_2')'(\underline{x}_1'M_{11}^{-1}M_{12}-\underline{x}_2')\beta_2'+2\underline{d}'KB'\underline{x}_1(\underline{x}_1'M_{11}^{-1}M_{12}-\underline{x}_2')\beta_2+\underline{d}'KT'B'\underline{x}_1\underline{x}_1'BTK\underline{d}$.

Therefore, $MSE[\hat{y}_m(\underline{x})]=\underline{x}_1'B(X'X)^{-}B'\underline{x}_1\sigma^2+\beta_2'P\beta_2+2\underline{d}'KQ\beta_2+\underline{d}'KSK\underline{d}$, where $P=(\underline{x}_1'M_{11}^{-1}M_{12}-\underline{x}_2')'(\underline{x}_1'M_{11}^{-1}M_{12}-\underline{x}_2')$, $Q=B'\underline{x}_1(\underline{x}_1'M_{11}^{-1}M_{12}-\underline{x}_2')$ and $S=T'B'\underline{x}_1\underline{x}_1'BT$.

Next, if the $MSE[\hat{y}_m(\underline{x})]$ is integrated over the region of interest R, we can further obtain that $V[\hat{y}_m]=\sigma^2 Tr[B(X'X)^{-}B'M_{11}]$ and $B[\hat{y}_m]=\underline{\beta}_2'P^*\underline{\beta}_2+\underline{d}'KS^*K\underline{d}$.

Therefore, we can obtain the result (2.2).

Q.E.D.

By using the *MBE*, the integrated squared bias of $\hat{y}_m(\underline{x})$ in (2.2) is decomposed into two parts. The first part, $\underline{\beta}_2'P^*\underline{\beta}_2$, is the result caused by model inadequacy and the last term,

$\underline{d}'KS^*K\underline{d}$, is the result caused by wild observations. When this is compared with the result of IMSE in Appendix, it is of interest to observe that the second term in $\beta[\hat{y}]$, $\underline{d}'KQ^*\underline{\beta}_2'$, becomes zero when the MBE is used. However, this term is not necessarily equal to zero when the least squares estimation (LSE) is used. (This will be shown in Appendix). Hence, the MBE is advantageous to the LSE when wild observations exist. Moreover, because each term of $B[\hat{y}_m]$ is a quadratic form, we easily achieve the more information. And by using the MBE, the first term in $B[\hat{y}_m]$ is minimized and $\underline{b}_m$ minimizes the integrated variance subject to minimum $B[\hat{y}_m]$ for any fixed design. Thus $\underline{b}_m$ makes smaller $IMSE$ than that by using the Box and Drapper approach, where in order to minimize the integrated squared bias they used the standard least squares estimators and the following condition ;

$$(X_1'X_1)^{-1}X_1'X_2=M_{11}^{-1}M_{12}.$$

Therefore, in order to reduce the effect of outliers proposed by a given aberration vector $\underline{d}$, we can regard the following condition as a robust design criterion to outliers. For a given $K\underline{d}$,

$$\text{Minimize } \underline{d}'KS^*K\underline{d} \quad \text{subject to } B(X'X)^-X'X=B. \tag{2.3}$$

Here, $B(X'X)^-X'X=B$ is a necessary condition for existence of the $\underline{b}_m$ (Ref. 6). Based on the results we have obtained, we propose a robust design criterion (2.3) for a given $K\underline{d}$. The design which minimizes (2.3) will be called the R-design. In the following sections we will treat further development of this criterion in order to obtain the simpler forms.

2.2 A Single Aberrant Observation in a Subset of Points

Suppose a design consists of s sets of experimental points, and a single aberrant observation exists at one set among s point sets. The sets will be called A_l with n_l elements for $1\leq l\leq s$.

For a single aberration of magnitude δ in the i^{th} observation, *i.e.* $k_i=1$ and $k_j=0$ for $j\neq i$ and $1\leq i\leq n$ in (2.1), $\underline{d}'KS^*K\underline{d}=\delta^2 s_{ii}^*$ where s_{ii}^* is the i^{th} diagonal element of S^*. When a single aberration of magnitude δ has equal probability of occurring at any of the n_l elements in A_l, we want to find the average value of $\underline{d}KS^*K\underline{d}$ over all K in the A_l set. By the following lemma, the average value will be obtained.

Lemma 2.2

Let $A_l=\{i \mid i_1\leq i\leq i_2\}$ with n_l elements where i_1 and i_2 are arbitrary observation numbers. When the magnitude of d_i is δ, the average of $\underline{d}'KS^*K\underline{d}$ over all K in A_l is

$$\overline{B}_1=\delta^2 T_r(S_l^*)/n_l,$$

where S_l^* is the $n_l\times n_l$ principal matrix of S^* with the $(i_1, \cdots, i_2)^{th}$ rows and columns.

proof

Let $Avg_K(\cdot)$ denote the average value of $(\cdot)$ with respect to K.

$$\overline{B}_1=Avg_K(\underline{d}'KS^*K\underline{d})=Avg_K[Tr(\underline{d}'KS^*K\underline{d})]=Avg_K[Tr(S^*K\underline{d}\underline{d}'K)]$$

$$=\delta^2 Avg_K[Tr(S^*KJK)]=\delta^2 Avg_K[Tr(\underline{1}'KS^*K\underline{1})],$$

where J is the $n\times n$ matrix with all elements 1's and $J=\underline{1}\underline{1}'$ with $\underline{1}'=(1, \cdots, 1)_{1\times n}$.

Let $\underline{1}'K=\underline{k}'=(k_1, k_2, \cdots, k_n)$, where k_i are defined in (2.1). Thus,

$$\bar{B}_l=\delta^2 Avg_{\underline{k}}[Tr(\underline{k}'S^*\underline{k})]=\delta^2 Avg_{\underline{k}}[\sum_{i\in A_l} s_{ii}^* k_i^2]=\delta^2\sum_{i\in A_l} s_{ii}^*/n_l=\delta^2 Tr(S_l^*)/n_l.$$

Q.E.D.

From the result of Lemma 2.2, $Tr(S_l^*)$ should be minimized to achieve robustness of $\underline{d}'KS^*K\underline{d}$ to a single aberrant observation for a fixed A_l.

The following Table 1 is obtained by Lemma 2.2. Table 1 ($c_1=2$ and $c_2=3$) is R-designs obtained from the rotatable equiradial designs with two circles, where p is the number of variables. The square region of interest represents $R=\{-1\leq x_i\leq 1 \text{ for all } i\}$. Note that n is the number of observations and n_1 and n_2 are the number of observations on the inner circle with radius r_1 and on the outer circle with radius r_2, respectively.

Table 1. R-designs over the square region of interest(p=2)

n	(I)	(II)
10	(5, 5, 0.44, 1.4142)*	(5, 5, 0.92, 1.4142)
11	(5, 6, 0.76, 1.4142)	(6,5, 0.62, 1.3140)
12	(5, 7, 0.76, 1.4142)	(7,5, 0.32, 1.0141)
13	(7,6, 0.80, 1.4142)	(7,6, 0.32, 1.0141)

* : (n_1, n_2, r_1, r_2)

(I) when one outlier exists on the outer circle.

(II) when one outlier exists on the inner circle.

We will treat further development of the proposed robust design criterion to reduce the effect of outliers when an outlier can occur in any point of a design. Such development can be more applicable in practice.

Corollary 1

When a single aberration of magnitude δ has equal probability of occurring at any of the n observations, the average of $\underline{d}'KS^*K\underline{d}$ over all K is

$$\bar{B}=\delta^2 Tr(S^*)/n=\delta^2\sum_i s_{ii}^*/n,$$

where s_{ii}^* is the i^{th} diagonal element of S^*.

From the result of *Corollary 1*, $Tr(S^*)$ should be minimized to achieve robustness of the *IMSE* $[\hat{y}_m]$ to an aberrant observation.

2.3 Serveral Aberrant Observations at Some Union of Subsets of Points

First of all, suppose that several aberrant observations exist at any union of sets of points with a single aberrant observation in each point set. When an aberrant observation of magnitude δ has equal probability of occurring at any n_l observation in the corresponding A_l, we want to find the average value of $\underline{d}'KS^*K\underline{d}$ with respect to K in $\cup_l A_l$, which denotes a union set of A_l's with one aberrant observation in each set. We can easily obtain the following lemma without proof by the same procedure as *Lemma 2.2*.

Lemma 2.3

$\cup_l A_l$ is the union of all sets with an aberrant observation. When the magnitude of aberration, δ, is equal, the average of $\underline{d}'KS^*K\underline{d}$ over all K in $\cup_l A_l$ is

$$\bar{B}_2=\delta^2 \sum_{(j,k)\in A_U} S_{(j,k)}{}^* / \prod_l \binom{n_l}{1}, \tag{2.4}$$

where $A_U=\{(j,k) \mid (j,k)$ *is an element of all possible combinations among* $A_l's\}$, and $S_{(j,k)}{}^*$ denotes the sum of all elements in the 2×2 principal matrix of S^*, which has only the j^{th} and k^{th} rows and the j^{th} and k^{th} columns of S^*.

From the result of *Lemma 2.3*, in order to obtain the R-designs according to the assumption of *Lemma 2.2*, $\bar{B}_2$ should be minimzed. It is equivalent to minimizing $\Sigma_{(j,k)\in A_U} S_{(j,k)}{}^*$ for fixed n_l's

Generally, we can consider the case of occurring different q_l's corresponding to A_l's, where q_l is the number of aberrant observations in A_l and $1\leq q_l \leq n_l$. For this case, in the formular of $\bar{B}_2$ in (2.4), only $\Pi_l\binom{n_l}{1}$ changes to $\Pi_l\binom{n_l}{q_l}$. Therefore, we can obtain the following lemma. Let $\cup_l A_l$ be the union of all sets with aberrations.

Lemma 2.4

When the number of aberration observations in some A_l's, q_l is different from one another, and the magnitude of aberrations is equal, δ, the average of $\underline{d}'KS^*K\underline{d}$ over all K in $\cup_l A_l$ is

$$\bar{B}_3=\delta^2\Sigma\Sigma_{(j,k)\in A_U} S^*_{(j,k)}/\prod_l\binom{n_l}{q_l}.$$

When several aberrant observations, q_l, exist at some corresponding A_l's, $\bar{B}_3$ should be minimized in order to obtain R-designs.

Those are represented as $A_1=\{1, 2, \cdots, n_1\}$ and $A_2=\{n_1+1, n_1+2, \cdots, n_1+n_2\}$, respectively. In the following Table 2, (q_1, q_2) denotes that q_1 outliers exist in A_1 and q_2 outliers exist in A_2.

Table 2. R-designs in rotatable equiradial designs corresponding for $q=2$ and 3 over the square region of interest (p=2)

(q_1, q_2)	10	11	12	13
(1, 1)	$(5, 5, 0.92, \sqrt{2})^*$	$(5, 6. 1.05, \sqrt{2})$	(5, 7, 0.95, 1.10)	(6, 7, 0.95, 1.02)
(1, 2)	$(5, 5, 0.88, \sqrt{2})$	(6, 5, 0.75, 1.22)	(7, 5, 0.30, 1.02)	(7, 6, 0.35, 1.02)
(2, 1)	$(5, 5, 0.92, \sqrt{2})$	$(5, 6. 1.05, \sqrt{2})$	$(5, 7, 1.00, \sqrt{2})$	$(6, 7, 1.00, \sqrt{2})$

$*$: (n_1, n_2, r_1, r_2)

We will also develop the robust design criterion to reduce the effect of outliers when outliers can occur in any point of a design with equal probability. If there are two or more aberrant observations, a similar conclusion can be deduced. We can obtain the following useful results for this case.

Corollary 2

If $d_i=\delta$ for all i, and there are $q(\geq 2)$ aberrant observations with equal probability of occuring at any of the n observations, the average of $\underline{d}KS^*K\underline{d}$ over all K is

$$\bar{B}_4=\delta^2\Sigma\Sigma_{(i,j)\in A_U} s_{ij}^*/w,$$

where s_{ij}^* is the $(i,j)^{th}$ element of S^*, $w=\binom{n}{q}$, and A_U is equal to that in *Lemma 2.3*.

Moreover, $\bar{B}_4$ can be expressed as follows:

$$\bar{B}_4=\delta^2[\gamma_1\sum_i s_{ii}^*+\gamma_2\Sigma\Sigma_{i\neq j}s_{ij}^*]/w,$$

where $\gamma_1=\binom{n_1-1}{q_1-1}$ denotes the occurrence frequency of each s_{ii}^* for any i and $\gamma_2=\binom{n_2-1}{q_2-1}$ denotes the occurrence frequency of each s_{ij}^* for $i\neq j$. $\bar{B}_4$ can be obtained by the following equation.

$$\bar{B}_4=\delta^2[\gamma_2\sum_i\sum_j s_{ij}^*+(\gamma_1-\gamma_2)\sum_i s_{ii}^*]/w. \tag{2.5}$$

From the result of *Corollary 2*, in order to reduce the effects of outliers, we should minimize the value of $\bar{B}_4$. The following lemma gives a useful tool in obtaining the minimum value of $\bar{B}_4$.

Lemma 2.5

When the *MBE* is utilized, the sum of all elements of S^* is 1.

Proof

Note that $X=(\underline{1}\mid X_R)$, where X_R is the remaining matrix without the first columm $\underline{1}$. From the necessary condition for existence of MBE, we can see that $B(X'X)^-X'(\underline{1}\mid X_R)=B$ and $[B(X'X)^-X'\underline{1}\mid B(X'X)^-X'X_R]=(I\mid M_{11}^{-11}M_{12})$.

Hence, we can easily consider the following relationship:

$$B(X'X)^-X'\underline{1}=(1,\ 0,\ \cdots,\ 0)'.$$

Since the sum of all elements of S^* can be represented as $\underline{1}'S^*\underline{1}$, we can complete the proof as follows:

$$\begin{aligned}\underline{1}'S^*\underline{1}&=\underline{1}'T'B'M_{11}BT\underline{1}=\underline{1}'X(X'X)^-B'M_{11}B(X'X)^-X'\underline{1}\\&=(1,\ 0,\ \cdots,\ 0)M_{11}(1,\ 0,\ \cdots,\ 0)'=m_{11}=1,\end{aligned}$$

where m_{11} is the first diagonal element of M_{11}.

By using the result of *Lemma 2.5*, we can find a simple form of the robust design criterion to minimize $\bar{B}_4$ for the case of several outliers.

Corollary 3

For the case of several outliers, $\overline{B}_4$ is minimized by minimizing $Tr(S^*)$ for a given $\underline{d}$.

proof

When the alternative form (2.5) of $\overline{B}_4$ is used, by *Lemma 2.5* $\overline{B}_4$ becomes as follows :

$$\overline{B}_4=\delta^2[\gamma_2+(\gamma_1-\gamma_2)\sum_i s_{ii}^*]/w.$$

Therefore, for a fixed n and q, $\overline{B}_4$ is minimized by minimizing $Tr(S^*)=\Sigma_i s_{ii}^*$.

Q.E.D.

3. Conclusions And Remarks

When outliers occur at a specific point sets and at any point of design with equal probability, the proposed robust design criterion is developed as simple forms in lemmas and corollaries in Section 2. In particular, we should note that when aberrations exist in the observations with equal probability, the proposed simpler criterion, $min\ Tr(S^*)$, is exactly the same as Karson, Manson and Hader's criterion, $min\ V\{[\hat{y}_m]/\sigma^2\}$ even though our approach is different from theirs. This $min\ Tr(S^*)$ differs from that of Box and Draper (1975), $min(\Sigma_i h_{ii}^2)$ diagonal element of the hat matrix $H=X(X'X)^{-1}X'$ and those of Herzberg and Andrews (1976) and Andrews and Herzberg(1979). The first different point is the choice of the estimation method, that is, $Tr(S^*)$ criterion is deduced by the *MBE* while their criteria are deduced by the *LSE*. The second is the choice of model, that is, they did not discuss model inadequacy. Another different point compared with that of Herzberg and Andrews (1976) is that once outliers have been identified, estimation of the unknown parameters based on the remaining data can be treated by assigning whether or not the i^{th} observation is rejected. And compared with that of Box and Draper(1975), it is the G-efficiency criterion used in the selection of a design to control the variance of the $\hat{y}$'s, $\hat{y}$ being the estimated value of the response function at a design point.

We believe that in constructing a design for response surface experiments, a design robustness should be considered as a design criterion in addition to rotatability, slope-rotatability, D-optimality and so on.

Appendix

When $\eta(\underline{x})$ is estimated by $\hat{y}(\underline{x})=\underline{x}_1'\underline{b}_1$ with $\underline{b}_1=(X_1'X_1)^{-1}X_1'\underline{y}$ but the true model $\eta(\underline{x})=\underline{x}_1'\underline{\beta}_1+\underline{x}_2'\underline{\beta}_2$ (for the complete set of n data points $\underline{\hat{y}}(\underline{x})=X_1\underline{b}_1$ and $\underline{\eta}(\underline{x})=X_1\underline{\beta}_1+X_2\underline{\beta}_2$), the *IMSE* of $\hat{y}(\underline{x})$ over the region R is expressed as follows :

$$IMSE[\hat{y}]=\sigma_2 Tr[(X_1'X_1)^{-1}M_{11}]+\underline{\beta}_2'P_1^*\underline{\beta}_2+2\underline{d}'KQ_1^*\underline{\beta}_2+\underline{d}'KS_1^*K\underline{d},$$

where $P_1^*=A'M_{11}A-M_{12}'A-A'M_{12}+M_{22}$, $Q_1^*=T_1'(M_{11}A-M_{12})$ and $S_1^*=T_1'M_{11}T_1$ with $A=(X_1'X_1)^{-1}X_1'X_2$ and $T_1=(X_1'X_1)^{-1}X_1'$.

proof

First, we have to obtain the $MSE[\hat{y}(\underline{x})]$. It can be shown that the variance part and the bias part as follows :

$Var[\hat{y}(\underline{x})]=Var(\underline{x}_1'\underline{b}_1)=\sigma^2\underline{x}_1'(X_1'X_1)^{-1}\underline{x}_1$, and $Bias^2[\hat{y}(\underline{x})]=[(x_1'A-x_2')\underline{\beta}_2+\underline{x}_1'T_1K\underline{d}]'[(\underline{x}_1'A-\underline{x}_2')\underline{\beta}_2+\underline{x}_1'T_1K\underline{d}]=\underline{\beta}_2'P_1\underline{\beta}_2+2\underline{d}'KQ_1\underline{\beta}_2+\underline{d}'KS_1K\underline{d}$,

where $P_1=A'\underline{x}_1\underline{x}_1'A-A'\underline{x}_1\underline{x}_2'-\underline{x}_2\underline{x}_1'A+\underline{x}_2\underline{x}_2'$, $Q_1=T_1'(\underline{x}_1\underline{x}_1'A-\underline{x}_1\underline{x}_2')$ and $S_1=T_1'\underline{x}_1\underline{x}_1'T_1$.

Note that $E[\hat{y}(\underline{x})]=\underline{x}_1'E(\underline{b}_1)=\underline{x}_1'(X_1'X_1)^{-1}X_1(X_1\underline{\beta}_1+X_2\underline{\beta}_2+K\underline{d})=\underline{x}_1'(\underline{\beta}_1+A\underline{\beta}_2+T_1K\underline{d})$.

Therefore, the $MSE[\hat{y}(\underline{x})]=\sigma^2\underline{x}_1'(X'X)^{-1}\underline{x}_1+\underline{\beta}_2'P_1\underline{\beta}_2+2\underline{d}'KQ_1\underline{\beta}_2+\underline{d}'KS_1K\underline{d}$. Next, if the $MSE[\hat{y}(\underline{x})]$ is integrated over the region of interest R, we can further obtain that $V[\hat{y}]=\sigma^2Tr[(X_1'X_1)^{-1}M_{11}]$ and $B[\hat{y}]=\underline{\beta}_2'P_1^*\underline{\beta}_2+2\underline{d}'KQ_1^*\underline{\beta}_2+\underline{d}'KS_1^*K\underline{d}$. Therefore, we can obtain the above equation of $IMSE[\hat{y}]$.

If Box and Drapper condition is satisfied, the second term of the above result becomes zero.

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