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Multi-response Designs Minimizing Model Inadequacies[1]

Whasoo Bae[2]

Abstract

This paper aims at selecting the multi-response design with r responses minimizing the bias error caused by fitting inadequate models to responses, where the first order models are fitted to p responses fearing the quadratic bias, while to other $r-p$ responses, the quadratic models are fitted fearing the cubic biases in the cuboidal region of interest. Under the assumption of symmetric design, by minimizing the criterion which represents the amount of error caused by fitting inadequate models, the optimum design was found to be the one having the design moments of second order and the fourth order as $1/3$ and $1/5$, respectively. Examples of the design meeting the required conditions are given for illustration.

Keywords : cuboidal region, bias error, design moment, multi-response design

1. Introduction

There are usually two types of problems concerning the choice of an experimental design, depending on the objectives of the investigation. We may wish (1) to estimate the parameters of a specified(known) relationship between the response and the input variables or (2) approximate (using some graduating function like polynomial) an unknown functional relationship within a specified region of interest, R, say.

The second case of design problem is examined here. The approximate relationship needs to represent the true or feared relationship satisfactorily in order to be used in further studies. Within the region of interest, it is needed to find a suitable size of a design which enables the fitted functional relationship to be close to the true relationship so that the fitted values and the true response values are as close as possible.

For example, assume that the true relationship is explained by a quadratic model in whole region of experiment, the region of operability, say O, but we do not know this. If we fit the first order model, then this one does not explain the true relationship in O. But there would

1) This work was supported by the Inje Scholarship Foundation in 2001.
2) Associate Professor, Department of Data Science, Inje University, Kimhae, 621-749, Korea.
E-mail : wbae@stat.inje.ac.kr

be a region within R, where the first order represent the relationship quite well. That region specified by a suitable design point set is needed to be found, so in that region, the first order explains the relationship successfully.

Box and Draper(1959, 1963) examined this type of design problem in the spherical region of interest by minimizing the gap between the fitted response values and the true values in the single response case. Two types of errors, the variance error and the bias error, were introduced, where the former was caused by the random fluctuation and the latter by fitting an inadequate model. The suitable design was shrunk to minimize the dominant bias error, while the design should be expanded to the experimental range for the dominant variance error. With equal amount of both the variance error and the bias error, the design had to be expanded slightly, about 10 % of the dominant bias error case. Thus the bias error was found to have large influence on design, when it was dominant. Draper and Lawrence(1965) discussed this type of problem considering the cubic region of interest.

Kim and Draper(1994) and Bae(1995) extended this problem to the multiple response case using the spherical region of interest. In Kim and Draper(1994), the first order model was fitted to all responses fearing the second order bias and Bae(1995) discussed about fitting the second order model to responses fearing that the true relationship might be represented as a cubic order model. The suitable design was found by minimizing a criterion represented by a matrix form, where the determinant, the trace, and the maximum eigen value of criterion were used for minimization. The multi-response case gave similar results to those in single response case for the dominant error as described in the first paragraph.

In this work, the multi-response design problem is reexamined in the cuboidal region of interest, assuming that the graduating function for each response is to be a first or second order polynomial. The suitable design is required to be chosen so that the fitted function for each response represents the true or feared functional relationship as closely as possible within the given region of interest, while the true or feared models are assumed to have higher orders than the fitted models by one. Also in finding the suitable design, the criterion used here is not a matrix form but a scalar form which describes the amount of error caused by fitting inadequate models.

In Section 2, the form of criterion is given and Section 3 shows the result after minimizing the criterion. The example of designs satisfying the conditions are given for illustration in Section 4 and finally, the concluding remarks are shown in Section 5.

2. The Criterion

Suppose that there are N observed values of r responses and each response is measured on k input variables, where the region of interest is assumed to be cuboidal and without loss of generality, we can set $-1 \leq x_i \leq 1$, for $i = 1, \cdots, k$, because it is always possible to transform every range to [-1, 1].

The first order models are to be fitted to p responses fearing the true model might be quadratic ones, while to other $r-p$ responses, the second order models are to be fitted fearing the cubic bias. It is also assumed that there are no common parameters among the responses so that the parameters can be estimated by using the original least squares method to each response independently as shown in Box and Tiao(1973) and Box and Draper(1965). Let $\hat{\boldsymbol{y}}(\boldsymbol{x})=(\hat{y}_{(1)}(\boldsymbol{x}), \hat{y}_{(2)}(\boldsymbol{x}),\cdots, \hat{y}_{(r)}(\boldsymbol{x}))'$ and $\boldsymbol{\eta}(\boldsymbol{x})=(\eta_{(1)}(\boldsymbol{x}), \eta_{(2)}(\boldsymbol{x}),\cdots, \eta_{(r)}(\boldsymbol{x}))'$ be $r\times 1$ vectors of fitted responses and true values, measured at a given input vector $\boldsymbol{x}=(x_1, x_2,\cdots,x_k)'$, respectively. Then,

$$\hat{y}_{(i)}(\boldsymbol{x})=\hat{\beta}_{0(i)}+\sum_{l=1}^{k}\hat{\beta}_{l(i)}x_l \tag{2.1}$$

and

$$\eta_{(i)}(\boldsymbol{x})=\beta_{0(i)}+\sum_{l=1}^{k}\beta_{l(i)}x_l+\sum_{l=1}^{k}\sum_{m\geq 1}^{k}\beta_{lm(i)}x_l x_m\ , \text{ for } i=1,2,\cdots,p \tag{2.2}$$

For $i=p+1,\cdots,r$,

$$\hat{y}_{(i)}(\boldsymbol{x})=\hat{\beta}_{0(i)}+\sum_{l=1}^{k}\hat{\beta}_{l(i)}x_l+\sum_{l=1}^{k}\sum_{m\geq 1}^{k}\widehat{\beta_{lm}}_{(i)}x_l x_m \tag{2.3}$$

and

$$\eta_{(i)}(\boldsymbol{x})=\beta_{0(i)}+\sum_{l=1}^{k}\beta_{l(i)}x_l+\sum_{l=1}^{k}\sum_{m\geq 1}^{k}\beta_{lm(i)}x_l x_m+\sum_{l=1}^{k}\sum_{m\geq 1}^{k}\sum_{n\geq m}^{k}\beta_{lmn(i)}x_l x_m x_n \tag{2.4}$$

Under this situation, the design is to be selected focusing on the case when the bias error is dominant. The criterion to be used here is represented as the amount of the expected standardized bias integrated over the region of interest, R, and adjusted by the number of observations N and weight Ω. The form of criterion is

$$\boldsymbol{J}=N\Omega\int_R[E\{(\hat{\boldsymbol{y}}(\boldsymbol{x})\}-\boldsymbol{\eta}(\boldsymbol{x})]'\boldsymbol{\Sigma}^{-1}[E\{\hat{\boldsymbol{y}}(\boldsymbol{x})\}-\boldsymbol{\eta}(\boldsymbol{x})]d\boldsymbol{x} \tag{2.5}$$

where $\boldsymbol{\Sigma}^{-1}=[Var\{(y_{(1)},\cdots,y_{(r)})'\}]^{-1}=\{\sigma^{ij},\ i,j=1,\cdots,r\}$ is the inverse of covariance matrix of responses and $\Omega=1/\int_R d\boldsymbol{x}$ in R and 0, otherwise. The covariance matrix of responses, which is usually unknown, is assumed to be known.

The design minimizing $\boldsymbol{J}$ is the one suitable for reducing the bias error caused by fitting inadequate models to responses as small as possible.

3. Results

If we assume the design to be symmetric for the informations to be given symmetrically, then the design moments of all odd orders are set to be zero so that

$$\sum_{u=1}^{N} x_{ul}^{d}/N = 0, \text{ where } d \text{ is an odd number for } \quad l=1,\cdots,k \tag{3.1}$$

and

$$\{\sum_{u=1}^{N} x_{ul}^{d_1} x_{u2}^{d_2} \ldots x_{uk}^{d_k}\}/N = 0, \text{ where at least one of } d_i's \text{ is odd.} \tag{3.2}$$

With the symmetry assumption, computing the criterion in (2.5), we could get that $J = B_1 + B_2 + B_{12}$, where

$$B_1 = N\Omega\sum_{i=1}^{p}\sum_{j=1}^{p}\sigma^{ij}\int_R\{E(\hat{y}_i)-\eta_i\}\{E(\hat{y}_j)-\eta_j\}d\boldsymbol{x},$$

$$B_2 = N\Omega\sum_{i=p+1}^{r}\sum_{j=p+1}^{r}\sigma^{ij}\int_R\{E(\hat{y}_i)-\eta_i\}\{E(\hat{y}_j)-\eta_j\}d\boldsymbol{x}\text{ , and}$$

$$B_{12} = 2N\Omega\sum_{i=1}^{p}\sum_{j=p+1}^{r}\sigma^{ij}\int_R\{E(\hat{y}_i)-\eta_i\}\{E(\hat{y}_j)-\eta_j\}d\boldsymbol{x} = 0,$$

because $\hat{y}_i$ for $i=1,\cdots,p$ has bias of the second order and $\hat{y}_j$ for $j=p+1,\cdots,r$ has bias of the third order so the multiplication of these two terms results in the order of odd order, where the design moments of all odd orders are assumed to be zero as in (3.1) and (3.2) because of symmetry. Hence the criterion in (2.5) is represented as a sum of two parts, which is $J = B_1 + B_2$.

In J, the weight function is set to be uniform, where $\Omega=1/\int_R d\boldsymbol{x}$ in R and 0, otherwise. Since the region of interest is cuboidal and $-1\le x_i\le 1$, for $i=1,\cdots,k$, $\Omega=1/\int_R d\boldsymbol{x}=1/2^k$. Also $\sigma^{ij}=\dfrac{(-1)^{i+j}|P|_{ij}}{|P|\,\sigma_i\sigma_j}$, where $|P|$ is the determinant of correlation matrix of responses P and $|P|_{ij}$ is the minor of σ_{ij} in $|P|$ and let $\dfrac{\beta_{lm(i)}}{\sigma_i/\sqrt{N}}=\alpha_{lm(i)}$ with σ_i as the standard deviation of the i^{th} response so that $\alpha_{lm(i)}$ represents the relative amount of $\beta_{lm(i)}$ to the variation in the i^{th} response.

First substituting these terms into B_1 in J, and if we complete the integration in B_1, we have

$$B_1 = \sum_{i=1}^{p} \sum_{j=1}^{p} \frac{(-1)^{i+j}\ |P|_{ij}}{|P|}\ \boldsymbol{\alpha}_{I(i)}{}' B_I\ \boldsymbol{\alpha}_{I(j)} \tag{3.3}$$

, where $\boldsymbol{\alpha}_{I(i)} = (\alpha_{11(i)}, \cdots, \alpha_{kk(i)}, \alpha_{12(i)}, \cdots, \alpha_{k-1,k(i)})'$ and $B_I = \begin{bmatrix} C1 & C2 \\ C3 & C4 \end{bmatrix}$

with

$$C1 = \begin{bmatrix} \lambda^2 + \frac{4}{45} & \lambda^2 & \cdot & \cdot & \cdot & \cdot & \lambda^2 \\ \lambda^2 & \lambda^2 + \frac{4}{45} & \lambda^2 & \cdot & \cdot & \cdot & \lambda^2 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \lambda^2 & \lambda^2 & \lambda^2 & \cdot & \cdot & \cdot & \lambda^2 + \frac{4}{45} \end{bmatrix} \tag{3.4}$$

as a $k \times k$ matrix with $\lambda = c - \frac{1}{3}$, where $c = \frac{\sum_{u=1}^{N} x_{ul}{}^2}{N}$ for $l = 1, \cdots, k$. Also

$$C2 = \begin{bmatrix} 0 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \cdot & 0 \end{bmatrix} \tag{3.5}$$

is a $k \times \binom{k}{2}$ matrix and $C3 = C2^t$, while

$$C4 = \begin{bmatrix} \frac{1}{9} & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & \frac{1}{9} & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & 0 & \frac{1}{9} \end{bmatrix} = \frac{1}{9}\ I_s \tag{3.6}$$

, where I_s is a $s \times s$ identity matrix with $s = \binom{k}{2}$.

Similarly, we have

$$B_2=\sum_{i=p+1}^{r}\sum_{j=p+1}^{r}\frac{(-1)^{i+j}\,|P|_{ij}}{|P|}\,\boldsymbol{\alpha}_{II(i)}{}'B_{II}\,\boldsymbol{\alpha}_{II(j)} \tag{3.7}$$

, where

$$\boldsymbol{\alpha}_{II(i)}=(\alpha_{111(i)},\alpha_{122(i)},\cdots,\alpha_{1kk(i)},\alpha_{222(i)},\alpha_{211(i)},\cdots,\alpha_{2kk(i)},\cdots,\alpha_{kkk(i)},\cdots,\\ \alpha_{k11(i)},\cdots,\alpha_{k,k-1,k-1(i)},\alpha_{123(i)},\cdots,\alpha_{k-2,k-1,k(i)})'$$

and

$$B_{II}=\begin{bmatrix}\Gamma_1 & \Gamma_2\\ \Gamma_3 & \Gamma_4\end{bmatrix} \tag{3.8}$$

with Γ_1 as a $k^2\times k^2$ block diagonal matrix where

$$\Gamma_1=\begin{pmatrix}\Gamma & \mathbf{0} & \cdot & \cdot & \cdot & \mathbf{0}\\ \mathbf{0} & \Gamma & \mathbf{0} & \cdot & \cdot & \mathbf{0}\\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\\ \mathbf{0} & \cdot & \cdot & \cdot & \mathbf{0} & \Gamma\end{pmatrix} \tag{3.9}$$

with

$$\Gamma=\frac{1}{3}\begin{bmatrix}\lambda_1{}^2+\frac{4}{(25)(7)} & \lambda_1\lambda_2 & \lambda_1\lambda_2 & \cdot & \cdot & \cdot & \lambda_1\lambda_2\\ \lambda_1\lambda_2 & \lambda_2{}^2+\frac{4}{(27)(5)} & \lambda_2{}^2 & \cdot & \cdot & \cdot & \lambda_2{}^2\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ \lambda_1\lambda_2 & \lambda_2{}^2 & \lambda_2{}^2 & \cdot & \cdot & \cdot & \lambda_2{}^2+\frac{4}{(27)(5)}\end{bmatrix} \tag{3.10}$$

and $\lambda_1 = \frac{e}{c} - \frac{3}{5}$ and $\lambda_2 = \frac{f}{c} - \frac{1}{3}$, where $\frac{\sum_{u=1}^{N} x_{ul}^{4}}{N} = e$ and $\frac{\sum_{u=1}^{N} x_{ul}^{2}\, x_{um}^{2}}{N} = f$, for $l \neq m$.
The matrix, Γ_2 is a $k^2 \times \binom{k}{3}$ zero matrix and $\Gamma_3 = \Gamma_2{}^t$, while $\Gamma_4 = \frac{1}{27} I_q$, where I_q is a $q \times q$ identity matrix with $q = \binom{k}{3}$.

Since both B_1 and B_2 are positive, it is possible that we do minimization of J sequentially to B_1 and B_2. As seen in (3.4) through (3.6), only the part C_1 in B_1 depends on the design moment so that $c = \frac{1}{3}$ makes B_1 minimized. In B_2, only the part Γ_1 contains the terms for design moments as shown in (3.9) and (3.10), so that B_2 is minimized when $\frac{e}{c} = \frac{3}{5}$ and $\frac{f}{c} = \frac{1}{3}$.

Combining the conditions for the second order design moment, $c = \frac{1}{3}$ and the fourth order one, $\frac{e}{c} = \frac{3}{5}$ and $\frac{f}{c} = \frac{1}{3}$, the proper design minimizing the model inadequacies can be described as the one satisfying $c = \frac{1}{3}$, $e = \frac{1}{5}$, and $f = \frac{1}{9}$.

4. Examples

Consider a point set with $(\pm a, \pm a, \cdots, \pm a)$ and $(\pm b, 0, \cdots, 0), \cdots, (0, \cdots, 0, \pm b)$, where there are n_0 center points $(0, 0, \cdots, 0)$. If we allow r_1 and r_2 replications on levels a and b, respectively, then there are $N = r_1(2^k) + r_2(2k) + n_0$ points.

For the case with $k = 1$, the optimum values of a and b satisfying the conditions, $c = \frac{2(r_1 a^2 + r_2 b^2)}{(2r_1 + 2r_2 + n_0)} = \frac{1}{3}$ and $e = \frac{2(r_1 a^4 + r_2 b^4)}{(2r_1 + 2r_2 + n_0)} = \frac{1}{5}$ are given in Table 1.

The optimum sizes of a and b having equal replications without center points are found to be .188 and .795, respectively, regardless of the number of replications. With $r_1 = r_2 = n_0$, we have .375 and .832 for a and b respectively, which is slightly larger size than those of the case without center points. Without replications, the maximum number of center points satisfying the conditions is 3 and the value of a increases as the number of center points increase, while the size of b increases up to 2 center points and decreases slightly after that. Table 1 illustrates the result for a and b with possible number of center points up to $N=$ 15. When there are more replications on one level than the other level, the design gets larger, compared to the case with same replications on each level.

Table 1. Optimum values of a and b with $k=1$

N	number of observations at					optimum values of	
	$-b$	$-a$	0	a	b	a	b
4	1	1	0	1	1	0.188	0.795
5	1	1	1	1	1	0.375	0.832
6	1	1	2	1	1	0.526	0.850
6	1	2	0	2	1	0.350	0.869
7	1	1	3	1	1	0.692	0.826
7	1	2	1	2	1	0.432	0.891
8	1	2	2	2	1	0.508	0.903
8	2	2	0	2	2	0.188	0.795
8	1	3	0	3	1	0.405	0.922
9	1	2	3	2	1	0.584	0.903
9	2	2	1	2	2	0.290	0.816
9	1	3	1	3	1	0.455	0.937
10	2	2	2	2	2	0.375	0.832
10	1	3	2	3	1	0.507	0.946
10	2	3	0	3	2	0.300	0.836
11	2	2	3	2	2	0.451	0.844
11	1	3	3	3	1	0.558	0.949
11	2	3	1	3	2	0.358	0.851
12	2	3	2	3	2	0.411	0.864
12	3	3	0	3	3	0.188	0.795
13	2	3	3	3	2	0.463	0.873
14	3	3	2	3	3	0.320	0.822
15	3	3	3	3	3	0.375	0.832

Table 2 shows the suitable values of a, b and n_0 in the cases with $k=2$, 3 and 4 satisfying the conditions for design moments $c=\dfrac{\{r_1(2^k a^2)+r_2(2kb^2)\}}{r_1(2^k)+r_2(2k)+n_0}=\dfrac{1}{3}$, $e=\dfrac{\{r_1(2^k a^4)+r_2(2kb^4)\}}{r_1(2^k)+r_2(2k)+n_0}=\dfrac{1}{5}$ and $f=\dfrac{\{r_1(2^k a^2)\}}{r_1(2^k)+r_2(2k)+n_0}=\dfrac{1}{9}$.

It is shown that the designs with $k\geq 2$ have bigger a and smaller b and also needs more center points than the designs with $k=1$. The optimum value of b increases under the same number of observations as we increase the number of inputs, k. With same situations regarding to replications, more center points are needed, while the size of a decreases and that of b increases as k increases.

Table 2. Optimum values of a, b and n_0 for $k \geq 2$

k	r_1	r_2	n_0	a	b
2	1	1	6.36	0.795	0.752
	1	2	8.52	0.869	0.691
	2	1	9.32	0.738	0.830
	2	2	12.71	0.795	0.752
3	1	1	11.19	0.769	0.782
	1	2	15.13	0.836	0.714
	2	1	16.33	0.718	0.868
	2	2	22.39	0.769	0.782
4	1	1	18.64	0.738	0.830
	1	2	25.42	0.795	0.752
	2	1	27.02	0.695	0.929
	2	2	37.28	0.738	0.830

5. Conclusions

The problem of selecting a multi-response design minimizing the model inadequacies was investigated in the cuboidal region of interest, where p responses were assumed to be fitted by the first order models fearing the quadratic bias and to the remaining $r-p$ responses, the quadratic models were fitted fearing the cubic bias.

The design was found by minimizing a criterion which specifies the mean squared standardized bias integrated over the region of interest, weighted by uniform weights and adjusted by the number of observations.

Assuming the symmetry of design, the suitable design which minimizes the model inadequacies in fitting the models of up to the second order fearing the bias of order higher than the fitted model by one, was found to be the one satisfying the conditions for the second order design moment as $c = \sum_{u=1}^{N} x_{ul}^2 / N = 1/3$ and the fourth design moments as

$e=\sum_{u=1}^{N} x_{ul}^{4}/N=1/5$ and $f=\sum_{u=1}^{N} x_{ul}^{2}\ x_{um}^{2}/N=1/9$. The correlations between the responses which appeared in this criterion seemed control the bias error in some way, but the amount controlled by the correlations did not have much influence in the dominant bias error case as shown in Kim and Draper(1994) and Bae(1995).

Applying these conditions to the design point set with $(\pm a,\ \pm a,\cdots,\pm a)$ and $(\pm b,\ 0,\cdots,0),\cdots,(0,\cdots,0,\pm b)$, including n_0 center points $(0,0,\cdots,0)$ with k input variables, it is shown that the designs need more center points as k increases. The designs for the case with $k\geq 2$ have bigger a and smaller b than the design with $k=1$ has. Also the optimum value of b increases. while the size of a decreases, as we increase k.

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