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A Study on a Basis for the Selection of a Design for Quadratic Model Fits Fearing a Cubic Bias in Multiple Response Case †

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ABSTRACT

In fitting a model, there always exists a discrepancy between the fitted model and the true functional relationship. In measuring this discrepancy, Box and Draper (1959) used the criterion dividing the discrepancy into two parts which are the bias error part and the variance error one in single response case. In this paper, an optimum design which makes these two types of errors as small as possible is found by extending the Box and Draper criterion to multiple response situation. Especially, a design is found to meet rotatability conditions when we fit a quadratic model to each response fearing cubic bias. Using the central composite design, an application of general results to a specific case is shown to help understanding the material.

KEYWORDS : Multiple response model, Variance error, Bias error, Rotatable design, Design moment.

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1. INTRODUCTION

Suppose we have decided to fit a general linear model to the response over a region of interest, say R. Then there would be a difference between the fitted model and the true functional relationship (or feared relationship) over the whole region of operability, say O.

Box and Draper(1959) used the weighted mean squared deviation from the true response averaged over the region R and normalized with respect to the number of observations and variance to measure the discrepancy. Box and Draper criterion divided the discrepancy into two parts which are called the bias error and the variance error. The former occurs from inadequacy of the fitted model and the latter from the sampling error. In 1963, they used this criterion in choosing a second order rotatable design for the single response case. This idea can be extended to the multi-response case in finding a criterion which measures the whole error amount from each response. If responses are not correlated, the amount of error can be computed by summing up errors which are computed separately, using Box and Draper criterion from each response. But it would not be correct, if the responses are correlated.

As mentioned in Khuri(1988) and Khuri and Cornell(1987), there are a lot of works relating the multiple response problem in many fields. But this type of response surface design problem has not been studied much in multiple-response situation. Kim and Draper(1994) discussed about choosing a design for straight line fits to two correlated responses.

The problem to be considered here is (1)to find a proper form of a criterion measuring the whole amount of discrepancy and (2)to obtain a suitable size of a rotatable design which minimizes errors, especially in fitting a quadratic model to each response fearing cubic terms as bias where there are several correlated responses.

In section 2, the model form and the notations in multi-response linear model are introduced and section 3 discusses the criterion measuring the discrepancy in multi-response case. In section 4, the choice of a suitable design which minimizes the errors presented in the criterion is examined and section 5 gives an application to a specific case using the central composite design. In section 6, concluding remarks are shown.

2. MODEL

Suppose that there are r responses measured on each of N experimental runs and that the models for the r responses depend on all of the experimental setting of k predictors. Then the model to be fitted over R is represented as

$$\mathbf{Y} \;=\; \mathbf{X}\beta \;+\; \epsilon, \tag{1}$$

,where $\mathbf{Y} = (\mathbf{y_1}, \cdots, \mathbf{y_r})$ with $\mathbf{y}_i = (y_{1i}, \cdots, y_{Ni})'$, $\mathbf{X} = (\mathbf{x}_1', \mathbf{x}_2', \cdots, \mathbf{x}_N')'$ with $\mathbf{x}_u' = (1, x_{u1}, \cdots, x_{uk}; {x_{u1}}^2, \cdots, {x_{uk}}^2\ ; x_{u1}x_{u2}, \cdots, x_{u(k-1)}x_{uk})'$, where $\beta = (\beta_1, , \cdots, \beta_r)$ with $\beta_i = (\beta_{0,i}, \beta_{1,i}, \cdots, \beta_{k,i};\ \beta_{11,i}, \cdots,\ \beta_{kk,i};\ \beta_{12,i}, \cdots,\ \beta_{(k-1)k,i})'$ for $i = 1, \cdots, r$ and $u = 1, \cdots, N$, where $\epsilon = (\epsilon_1, \cdots, \epsilon_r)$ with $\epsilon_i = (\epsilon_{1i}, \cdots, \epsilon_{Ni})'$ is an $N \times r$ error matrix and we assume that there are no common parameters among the functions of responses. In fitting the model in multiple response situation, the determinant criterion, which Box and Draper(1965) suggested, minimizing $|\epsilon'\epsilon|$, could be used. With no common parameter assumption, minimizing $|\epsilon'\epsilon|$, is exactly the same as the ordinary least squares estimation to each response separately in fitting the model when we have the same design structure for each response(see Box and Tiao(1973, pp.438-440)).

Assuming that the responses are correlated, the variance-covariance matrix of each row vector of ϵ is Σ, where $\Sigma = (\rho_{ij}\sigma_i\sigma_j, i, j = 1, \cdots, r)$ with $\rho_{ij} = 1$ for $i = j$ and $\mathrm{cov}(\epsilon_{ui}, \epsilon_{vj}) = \rho_{ij}\sigma_i\sigma_j$ if $u = v$, 0 otherwise for any $i, j = 1, \cdots, r$ and $u, v = 1, \cdots, N$. Hence $\mathrm{Var}(\epsilon) = \Sigma \otimes \mathbf{I}_\mathrm{N}$, an $Nr \times Nr$ matrix, where $\otimes$ means Kronecker product and $\mathbf{I}_\mathrm{N}$ is an $N \times N$ identity matrix.

If we assume that the true or "feared" relationship over the whole region of operability, say O, is represented as a quadratic model to each response,then

$$\mathrm{E}(\mathbf{Y}) \;=\; \eta \;=\; \mathbf{X}\beta \;+\; \mathbf{Z\Gamma}, \tag{2}$$

,where $\eta = (\eta_1, \cdots, \eta_r)$ with $\eta_i = (\eta_{1i}, \cdots, \eta_{Ni})'$, where $\mathbf{Z} = (\mathbf{z_1}', \cdots, \mathbf{z_N}')'$ with $\mathbf{z_u}' = ({x_{u1}}^3, x_{u1}{x_{u2}}^2, \cdots, x_{u1}{x_{uk}}^2; \cdots; {x_{uk}}^3, x_{uk}{x_{u1}}^2, \cdots, x_{uk}{x_{u(k-1)}}^2; x_{u1}x_{u2}x_{u3}, \cdots, x_{u(k-2)}x_{u(k-1)}x_{uk})'$, and where $\Gamma = (\gamma_1, \cdots, \gamma_r)$ with $\gamma_i = (\beta_{111,i}, \beta_{122,i}, \cdots, \beta_{1kk,i}\ ; \cdots; \beta_{kkk,i}, \beta_{k11,i}, \cdots, \beta_{k(k-1)(k-1),i}; \beta_{123,i}, \cdots, \beta_{(k-2)(k-1)k,i})'$ for $i = 1, \cdots, r$ and $u = 1, \cdots, N$.

Some designs are preferred by the experimenter because they provide informations symmetrically. Hence the choice of the region of interest R, is usually made to be symmetric. In this work, we shall choose R as a spherical region of unit radius, a choice that is frequently made, sensible and convenient. Thus the center of R is at $(0,\cdots,0)$ and all points on or within the region satisfy

$$\sum_{j=1}^{k} {x_j}^2 \leq 1 \quad . \tag{3}$$

For this region,

$$\int_R {x_1}^{\delta_1} {x_2}^{\delta_2} \cdots {x_k}^{\delta_k} dx_1 \cdots dx_k \;=\; \frac{\Gamma\left(\frac{\delta_1+1}{2}\right)\Gamma\left(\frac{\delta_2+1}{2}\right)\cdots\Gamma\left(\frac{\delta_k+1}{2}\right)}{\Gamma\{\frac{\sum_j(\delta_j+1)}{2}+1\}} \tag{4}$$

unless any δ_j is odd where the value of integral is zero and $\Gamma(1/2) = \sqrt{\pi}$ and $\Gamma(n) = (n-1)!$.

There is no restriction that all the experimental runs need to be within R in order to explore R. That is,some or all runs might be inside, and/or outside R.

3. MODEL

3.1 Rotatability Conditions

The design we intend to consider is a second order design, because we fit the second order fearing the third order bias. Especially, the second order design minimizing the bias is shown to be a rotatable design(see Myers(1971, p.214)). Hence we will now consider selecting the design from the class of the second order rotatable design which minimizes the variance error and the bias error simultaneously. Therefore a design needs to satisfy the following conditions(see Box and Draper(1987, p.489));

(1) $N^{-1}\sum_{u=1}^{N} {x_{u1}}^{\delta_1} {x_{u2}}^{\delta_2} \cdots {x_{uk}}^{\delta_k} \;=\; 0$, if any δ_l is odd, for $\sum_{l=1}^{k} \delta_l \leq 4$,

(2) $N\lambda_2 \;=\; \sum_{u=1}^{N} {x_{ul}}^2$,

(3) $3N\lambda_4 \;=\; \sum_{u=1}^{N} {x_{ul}}^4 \;=\; 3\sum_{u=1}^{N} {x_{ul}}^2 {x_{um}}^2$, for $l \neq m = 1,\cdots,k$.

The condition (2) and (3) serve to define λ_2 and λ_4.

3.2 The Form of Criterion

Let $\hat{\mathbf{y}}(\mathbf{x})$ and $\eta(\mathbf{x})$ be defined, respectively as fitted values of $\mathbf{Y}$ and the corresponding true mean values at the point $\mathbf{x} = (1, x_1, \cdots, x_k)'$. Then we want to choose the design to minimize

$$\mathbf{J} = \mathrm{N}\mathbf{\Sigma}^{-1} \int_{\mathrm{O}} \mathrm{w}(\mathbf{x})\ \mathrm{E}\{\hat{\mathbf{y}}(\mathbf{x}) - \eta(\mathbf{x})\}'\{\hat{\mathbf{y}}(\mathbf{x}) - \eta(\mathbf{x})\}\ d\mathbf{x}, \tag{5}$$

where $w(\mathbf{x})$ is a weight function and $d\mathbf{x} = dx_1 \cdots dx_k$. For the weight function, there could be various types of weight functions to give varying importance to some or other parts of the whole operable region. In this work, we shall consider a uniform weight function within R and zero outside it, because it is desired to weight response equally within R. Hence, $w(\mathbf{x}) = \Omega = 1/\int_R d\mathbf{x}$ in R and 0 elsewhere. In (5), the multiplication factor $N\Sigma^{-1}$ is the natural extension of the N/σ^2 factor for the multivariate case. The form of $\mathbf{J}$ can be written as following;

$$\begin{aligned} \mathbf{J} &= \mathrm{N}\Omega \int_{\mathrm{R}} \mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}\ \mathrm{d}\mathbf{x}\ \ \mathbf{I}_r \\ &+ \mathrm{N}\Omega\mathbf{\Sigma}^{-1} \int_{\mathrm{R}} \mathbf{\Gamma}'\{\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Z} - \mathbf{z}'\}'\{\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Z} - \mathbf{z}'\}\mathbf{\Gamma}\ \mathrm{d}\mathbf{x} \\ &= \mathbf{V} + \mathbf{B}, \end{aligned} \tag{6}$$

where $\mathbf{I}_r$ is an $r \times r$ identity matrix. From this, we see that the criterion $\mathbf{J}$, which is an $r \times r$ matrix, can be represented by the sum of the contributions from the two types of errors where $\mathbf{V}$ explains the variance error and $\mathbf{B}$ the bias error.

As shown in (6), the discrepancy between the fitted model and the feared one explained in $\mathbf{J}$, is divided into two parts in matrix form. How can one "minimize $\mathbf{J}$ " which is an $r \times r$ matrix ? Hence the trace of $\mathbf{J}$, say $tr(\mathbf{J})$, is chosen among possible choices. (Computations on the determinant of $\mathbf{J}$, and on the maximum eigen value of $\mathbf{J}$, showed very similar results.)

After completion of the appropriate calculations with rotatability conditions having fifth order design moments zero, the form of $\mathbf{V}$ is

$$\begin{aligned}
\mathbf{V} &= \mathrm{N}\Omega \int_{\mathrm{R}} \mathrm{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathrm{x}\ \mathrm{dx}\ \ \mathbf{I}_{\mathrm{r}} \\
&= [\frac{1}{\lambda_2} + \frac{3(k-1)}{2(k+4)\theta\lambda_2}]\mathbf{I_r} \\
&+[\frac{(k+2)(k+4)\theta\lambda_2 + 3 - 2(k+4)\theta}{(k+4)\lambda_2((k+2)\theta - 3k\lambda_2)}]\mathbf{I_r} \\
&= v(\lambda_2,\ \theta)\ \mathbf{I_r},
\end{aligned} \tag{7}$$

where $\theta = 3\lambda_4 / \lambda_2$ and $\mathbf{I_r}$ is an $r \times r$ identity matrix. We see that $\mathbf{V}$ depends on θ and λ_2 as far as the design moments are concerned. On the other hand, the form of $\mathbf{B}$ is represented as follows;

$$\begin{aligned}
\mathbf{B} &= \mathrm{N}\Omega\mathbf{\Sigma}^{-1} \int_{\mathrm{R}} \mathbf{\Gamma}'\{\mathrm{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Z} - \mathbf{z}'\}'\{\mathrm{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Z} - \mathbf{z}'\}\mathbf{\Gamma}\ \mathrm{dx} \\
&= N\mathbf{\Sigma}^{-1}\Gamma'\{\mathbf{A}'\Omega \int_R \mathbf{xx'dxA} - 2\Omega \int_R \mathbf{zx'dx} + \mathbf{\Omega} \int_{\mathbf{R}} \mathbf{zz'dx}\}\mathbf{\Gamma} \\
&= N\mathbf{\Sigma}^{-1}\Gamma'\mathbf{Q}\Gamma
\end{aligned} \tag{8}$$

,where $\mathbf{A} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Z}$ is an alias matrix and

$$\begin{aligned}
\mathbf{Q} &= \mathbf{A}'\Omega \int_R \mathbf{xx'dxA} - 2\Omega \int_R \mathbf{zx'dx} + \mathbf{\Omega} \int_{\mathbf{R}} \mathbf{zz'dx} \\
&= \begin{pmatrix} \mathbf{Q_1} & & & & \\ & \mathbf{Q_1} & & & \\ & & \ddots & & \\ & & & \mathbf{Q_1} & \\ & & & & \mathbf{Q_2} \end{pmatrix}
\end{aligned} \tag{9}$$

with

$$\mathbf{Q_1} = \begin{pmatrix} C & D & D & \dots & D \\ D & E & F & \dots & F \\ D & F & E & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & F \\ D & F & \dots & F & E \end{pmatrix}$$

and

$$\mathbf{Q_2} = \mathbf{I_q}/(k+2)(k+4)^2(k+6) = w\mathbf{I_q},$$

where $q = k(k-1)(k-2)$ and $\mathbf{I_q}$ is a $q \times q$ identity matrix. If we define

$$U = \{\theta - 3/(k+4)\}/9(k+2), \quad W = 1/(k+2)(k+4)^2(k+6);$$

then $C = 9U + 6(k+1)W$, $D = 3U - 6W$, $E = U + 2(k+3)W$, $F = U - 2W$.
Hence

$$\mathbf{B} = |\mathbf{\Sigma}|^*\{\mathrm{B_{ij}} \ \ i,\ j = 1, \cdots, r\}, \quad \text{an } r \times r \text{ matrix,} \tag{10}$$

, where

$$\begin{aligned}\Sigma^{-1} &= \prod_{i=1}^{r} \sigma_i{}^2 |\Sigma|^{-1}\{\sigma^{ij}\} \\ &= |\Sigma|^*\{\sigma^{ij*}\} \text{ for } i,j = 1,\cdots,r,\end{aligned} \tag{11}$$

and

$$\begin{aligned}\mathrm{B_{ij}} &= \sum_{s=1}^{r} N|\Sigma|^*\sigma^{is*}\Gamma'\mathbf{Q}\Gamma \\ &= |\Sigma|^* \sum_{s=1}^{r} [P_{sj}b(\theta) + \frac{(k+4)Q_{sj} - 2P_{sj}}{(k+2)(k+4)^2(k+6)}],\end{aligned} \tag{12}$$

with

$$\begin{aligned}P_{sj} = &(3\alpha_{111,s} + \alpha_{122,s} + \cdots + \alpha_{1kk,s})(3\alpha_{111,j} + \alpha_{122,j} + \cdots + \alpha_{1kk,j}) \\ &+ \quad \cdots \quad + \\ &(3\alpha_{kkk,s} + \alpha_{k11,s} + \cdots + \alpha_{k(k-1)(k-1),s})(3\alpha_{kkk,j} + \alpha_{k11,j} \\ &+ \quad \cdots \quad + \alpha_{k(k-1)(k-1),j})\end{aligned} \tag{13}$$

and

$$\begin{aligned}Q_{sj} = \ &2(3\alpha_{111,s}\alpha_{111,j} + \alpha_{122,s}\alpha_{122,j} + \cdots + \alpha_{1kk,s}\alpha_{1kk,j}) \\ &+ \quad \cdots \quad + \\ &2(3\alpha_{kkk,s}\alpha_{kkk,j} + \alpha_{k11,s}\alpha_{k11,j} + \cdots + \alpha_{k(k-1)(k-1),s}\alpha_{k(k-1)(k-1),j}) \\ &+ (\alpha_{123,s}\alpha_{123,j} + \cdots + \alpha_{(k-2)(k-1)k,s}\alpha_{(k-2)(k-1)k,j}),\end{aligned} \tag{14}$$

, where $b(\theta) = \frac{\{\theta - 3/(k+4)\}^2}{9(k+2)}$ and $\alpha_{lmn,i} = \frac{\beta_{klm,i}}{\sigma_i/\sqrt{N}}$, for $l,m,n = 1,\cdots,k$ and $i,j = 1,\cdots,r$.

Hence the form of the $tr(\mathbf{J})$ criterion is written as following,

$$tr(\mathbf{J}) = rv(\lambda_2, \theta) + tr(\mathbf{B}) \tag{15}$$

, where $v(\lambda_2, \theta)$ is as in (7) and

$$\begin{aligned} tr(\mathbf{B}) &= |\mathbf{\Sigma}|^* \sum_{\mathbf{i=1}}^{\mathbf{r}} \sum_{\mathbf{s=1}}^{\mathbf{r}} [\mathbf{P_{si} b(\theta)} + \{(\mathbf{k+4})\mathbf{Q_{si}} - \mathbf{2P_{si}}\}/(\mathbf{k+2})(\mathbf{k+4})^2(\mathbf{k+6})] \\ &= Pb(\theta) + \{(k+4)Q - 2P\}/(k+2)(k+4)^2(k+6) \end{aligned} \tag{16}$$

with $P = \sum_{i=1}^{r} \sum_{s=1}^{r} |\Sigma|^* P_{si}$ and $Q = \sum_{i=1}^{r} \sum_{s=1}^{r} |\Sigma^*| Q_{si}$.

Finally, $tr(\mathbf{J})$ is shown to be divided into two parts, which are the variance error part and the bias error one. So (15) is wrritten as following;

$$tr(\mathbf{J}) = v^* + b^* \tag{17}$$

, where $v^* = r\ v(\lambda_2, \theta)$ represents the variance error part and $b^* = tr(\mathbf{B})$ the bias error one.

3.3 Minimization of the $tr(\mathbf{J})$ Criterion

Using the form founded in section 3.2, the aim is to find a proper design which makes the gap, which can be measured using the form in (15), between the fitted model and the feared one as small as possible

In order to minimize (15), we fix θ, differentiate (15) with respect to λ_2, equate to 0, and we then have

$$\frac{\partial}{\partial \lambda_2} tr(\mathbf{J}) = r \frac{\partial}{\partial \lambda_2} v(\lambda_2, \theta) = 0. \tag{18}$$

Solving (18) for λ_2, gives

$$\lambda_2 = \theta\left[\frac{-3k\{2(k+4)\theta + 3(k+1) + \sqrt{(*)}\}}{3\{2\theta^2(k+2)(k+4) - 6k(k+4)\theta - 9k(k-1)\}}\right], \tag{19}$$

where

$$(*) = 6[\{2(k+4)\theta + 3(k+1)\}\{(k+2)^2(k+4)\theta^2 - 6k(k+4)\theta + 9k\}].$$

If we substitute in (15) for λ_2 from (19), differentiate with respect to θ, equate to 0, we obtain

$$\frac{\partial\nu(\lambda_2,\theta)}{\partial\lambda_2}\frac{d\lambda_2}{d\theta} + \frac{\partial\nu(\lambda_2,\theta)}{\partial\theta} + \frac{dtr(\mathbf{B})}{d\theta} = 0 ,$$

or equivalently,

$$\frac{\partial\nu(\lambda_2,\theta)}{\partial\theta} + \frac{dtr(\mathbf{B})}{d\theta} = 0, \quad \text{since} \quad \frac{\partial\nu(\lambda_2,\theta)}{\partial\lambda_2} = 0 \tag{20}$$

, where

$$\frac{\partial\nu(\lambda_2,\theta)}{\partial\theta} = \frac{-3}{(k+4)\lambda_2}\left[\frac{(k-1)}{2\theta^2} + \frac{k(k+4)\lambda_2\{(k+2)\lambda_2-2\}+(k+2)}{(k+2)\theta-3k\lambda_2{}^2}\right]$$

, and

$$\frac{dtr(\mathbf{B})}{d\theta} = \frac{2}{9(k+2)}\{\theta - \frac{3}{(k+4)}\}P_{tr}$$

, where P in the $tr(\mathbf{J})$ criterion is denoted by P_{tr}.

So (20) implies that

$$P_{tr} = \frac{27r(k+2)}{2\lambda_2\{(k+4)\theta-3\}}\left[\frac{(k-1)}{2\theta^2} + \frac{k(k+4)\lambda_2\{(k+2)\lambda_2-2\}+(k+2)}{\{(k+2)\theta-3k\lambda_2\}^2}\right] \tag{21}$$

, where $\lambda_2 = \lambda_2(\theta)$ as given in (19).

Hence, with specified values of P_{tr} , we can always get the optimum value of θ using (21) in the $tr(\mathbf{J})$ criterion. Via these values of θ, the optimum values of λ_2 can be obtained from (19).

4. RESULTS

4.1 General Results

With specified values of α's and ρ's, P_{tr} is determined and as shown in section 3.3, the optimum values of θ and λ_2 are obtained. That is, the design is depending on the second order and the fourth order of design moments. If we let $\lambda = \theta/\lambda_2 = 3\lambda_4/\lambda_2{}^2$, then λ will estimate the kurtosis of the design.

When the α's are too small or too large(which leads to either the variance error or bias error dominant cases, respectively), the optimum design size is not sensitive to changes in the correlations.

FIGURE 4.1 shows the changes in the optima of λ and $\sqrt{\lambda_2}$ depending on the specified values of P_{tr} for the various values of r's and k's. From FIGURE 4.1, we see that with the same value of k's, we have slightly bigger values of optimum $\sqrt{\lambda_2}$ and λ as we increase the number of responses. On the other

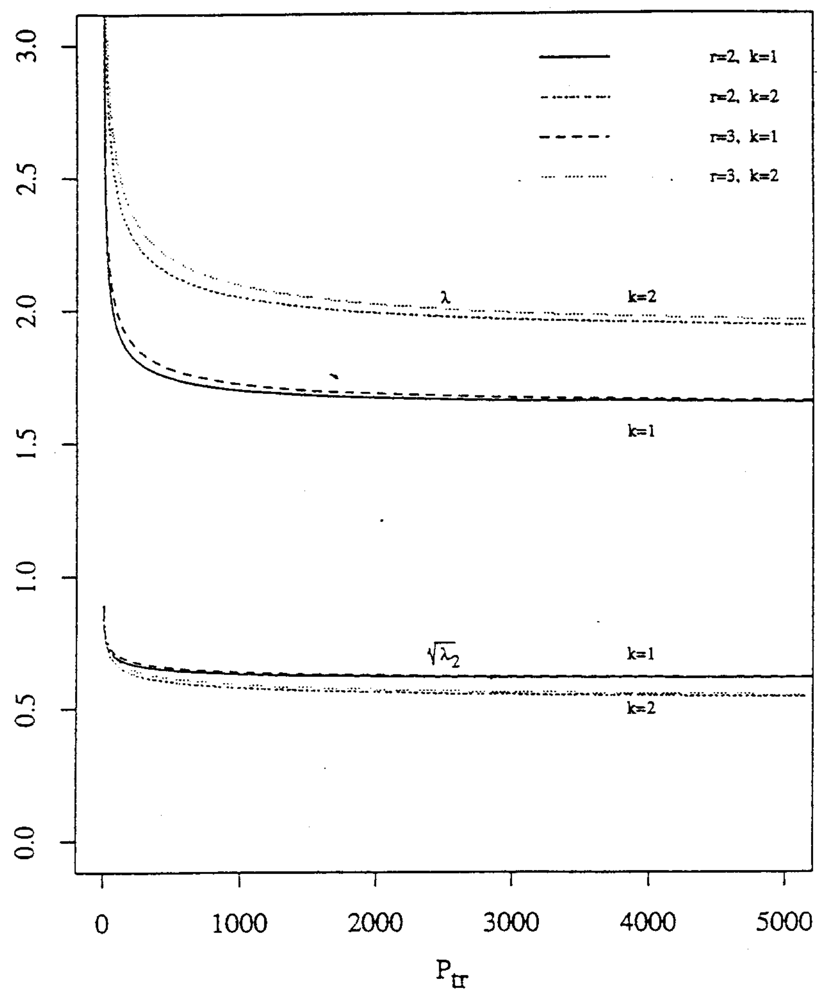

Figure 4.1. Change of optimum $\sqrt{\lambda_2}$ and λ as P_{tr} change

hand, with the same number of responses, we have smaller values of $\sqrt{\lambda_2}$ and bigger values of λ as we increase the number of predictors, by a much wider margins.

The effect of correlations can be checked for the specified number of responses. Hence, in order to examine the influence of correlations, the case with $r = 2$ and $k = 2$ is studied in the next section.

4.2 The Case with $r = 2$ and $k = 2$

To examine the sensitivity of the size of design with respect to changes in the correlation, we have chosen $|\alpha| \leq 1$. By the definition of the α's, this specification of the α's means that the ratio of each coefficient of the cubic curvature to the variation of $\bar{y}_i$, which is the mean of the i^{th} response, is less than or equal to 1 in absolute value. When the α's are such that $|\alpha| \leq 1$, even with the maximum value of P_{tr}, the ratio of variance error and the bias one, v^*/b^*, lies between 2 and 6 for various values of correlations. This means that the variance error contribution is 2 to 6 times as big as the bias error contribution. For a wider range of the α's, this ratio will be reduced. For example, with $|\alpha| \leq 2$, v^*/b^* ranges between 1.5 and 4 when the P_{tr} attains maximum values.

Table 4.1 shows the optimum values of $\sqrt{\lambda_2}$ and λ with respect to the changes in the correlation, assuming $\alpha = 1$. As ρ moves towards the positive side, bias gets smaller so that the design gets larger.

Table 4.1. Optimum Values of $\sqrt{\lambda_2}$ and λ as ρ change

ρ	P_{tr}	$\sqrt{\lambda_2}$	λ
-0.9	640	0.593	2.102
-0.7	213	0.632	2.276
-0.5	128	0.654	2.386
-0.3	91	0.668	2.464
-0.1	71	0.680	2.523
0.0	64	0.684	2.558
0.1	58	0.691	2.595
0.3	49	0.699	2.640
0.5	43	0.705	2.676
0.7	38	0.712	2.720
0.9	34	0.718	2.755

5. AN APPLICATION

Suppose that there are $r = 2$ and $k = 2$. Suppose further that for each response, we fit a second order model over R, which is the circular region with unit radius, but fear that cubic bias may be present. If we employ the central composite design, then the design points consist of three portions, namely, the cube portion, the star portion, and the center points. With $k = 2$, these design points are specified as $(s,\ s)$, $(s, -s)$, $(-s,\ s), (-s, -s)$, $(\sqrt{2}s,\ 0)$, $(-\sqrt{2}s, 0)$, $(0, \sqrt{2}s)$, $(0,\ -\sqrt{2}s)$, and $(0,\ 0)$, $\cdots, (0,\ 0)$, respectively. If we define the number of center points by n_0, then the total number of design points is $N = 8 + n_0$. Then

$$\lambda_2 = 8s^2/(8 + n_0) \tag{22}$$

$$3\lambda_4 = 12s^4/(8 + n_0) \tag{23}$$

So, using the values of λ_2 and λ_4, we can determine the proper values for s and n_0.

If we consider the case when the α's are all 1, then the values of optimum λ and $\sqrt{\lambda_2}$ shown in Table 4.1 can be used in finding the values for s and n_0. Since $\lambda = 3\lambda_4/\lambda_2{}^2$, using (22) and (23), we obtain

$$s = \sqrt{(2/3)\lambda_2\lambda} \quad \text{and} \quad \mathrm{n}_0 = (16/3)\lambda - 8 \tag{24}$$

By (24) and the results of Table 4.1, the values for s and n_0 are thus obtained and Table 5.1 shows these results as ρ varies.

From Table 5.1, we see that as the bias gets larger(ρ moves to the negative side) the design radius, s, gets smaller and we need fewer center points.

We see that, as we expect less bias error, we add more center points to provide a better estimate of the error variation and we spread the other points further from the origin, even outside of R. When the bias error is the main contribution to the error, however, the design contracts into R and we need only a few center points (3 or 4). When the bias error is dominant, the optimum values of s and n_0 are .578 and 2, respectively.

Table 5.1 Optimum Values of n_0 and s as ρ changs ($\alpha = 1$)

ρ	n_0	s
-0.9	3	0.702
-0.7	4	0.789
-0.5	5	0.826
-0.3	5	0.856
-0.1	5	0.883
0.0	6	0.894
0.1	6	0.909
0.3	6	0.927
0.5	6	0.942
0.7	7	0.959
0.9	7	0.973

6. CONCLUDING REMARKS

The optimum design was found by minimizing $tr(\mathbf{J})$, where $\mathbf{J} = \mathbf{V} + \mathbf{B}$. The correlations of the responses appear only in matrix **B**, the bias error part so that they influence only the bias error, interacting with the values of the α's. The influence of the correlation coefficients become weaker and weaker as the design situation becomes close to either the variance error dominant one or the bias error dominant one but, except these two extreme cases, the correlation coefficients influence the bias, which in turn affect the size of the design.

Using designs satisfying the conditions of second order rotatability, we determined the optimum size of the second order and the fourth order design moments, λ_2 and λ_4. The optimum design size can be specified using $\sqrt{\lambda_2}$ and $\lambda = 3\lambda_4/\lambda_2{}^2$, which shows the kurtosis of the design.

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