EXPERIMENTAL DESIGNS FOR ESTIMATING THE SLOPE OF SECOND ORDER POLYNOMIAL RESPONSE SURFACES

by

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TABLE OF CONTENTS

1. INTRODUCTION

This thesis 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, η , and several independent variables, $x_1, x_2, \ldots, x_p$, over some region of experimental interest in the space of the quantitative factors. The relationship could be expressed generally as

$$\eta = f(x_1, x_2, \ldots, x_p, \theta_1, \theta_2, \ldots, \theta_r) \tag{1}$$

where θ_i's are unknown parameters which must be estimated by experimental data.

The response relationship is usually interpreted geometrically as a response surface in a space of dimension $p + 1$ where the co-ordinates are the $p + 1$ variables, $x_1, x_2, \ldots, x_p$ and η . To explore the response relationship N observations of the response η are taken in the region of experimental operability at a set of N corresponding levels of each x_i ; these levels constituting an experimental design. The data are then used to fit an equation, $\hat{y}$, intended to estimate η over the region of interest. The region of interest (which will be denoted by R) is not necessarily the same as the region of operability (which will be denoted by RO) in which it is feasible to perform trials. Usually R is smaller than or equal to RO . It is convenient to transform the actual experimental variables so that their origin $(0, 0, \ldots, 0)$ is at the center of the region of interest, R , and so that R is either the p-dimensional cube defined by $-1 \leq x_i \leq 1$ or the unit sphere defined by $\sum_{i=1}^{p} x_i^2 \leq 1$.

If the true function form $\eta = f(\underline{x}, \underline{\beta})$ is unknown, as is often the case, the relationship may be approximated by the low order terms in the Taylor series expansion of equation (1), which might be expressed as

$$\eta = \beta_0 + \sum_{i=1}^{p} \beta_i x_i + \sum_{i \leq j=1}^{p} \beta_{ij} x_i x_j + \sum_{i \leq j \leq k=1}^{p} \beta_{ijk} x_i x_j x_k + \ldots .$$

A first order approximation is obtained by disregarding all terms beyond the first summation sign; a second order approximation is obtained by adding the second summation sign to the first order approximation, etc. Box and his co-workers have found that in most experimental situations the first or the second order approximation will be adequate for practical purposes. The coefficients of such polynomials are then the unknown parameters, which are usually estimated by least squares methods from experimental data. Various properties of the resulting fitted polynomials have been discussed; in particular, those properties which mainly depend on the choice of the experimental design.

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 of the fitted polynomial as a whole. One of the most popular variance criteria at present, along with the D-optimality criterion, is the concept of rotatability due to Box and

Hunter (5). The rotatable design is independent of its orientation in the sense that the variance of the fitted response, $\hat{y}$, at a point $\underset{\sim}{x} = (x_1, x_2, \ldots, x_p)$ in the factor space depends only on the distance from $\underset{\sim}{x}$ to the center of the design. Box and Hunter have derived a group of rotatable designs for fitting second order polynomials.

In later work, the question of bias due to inadequacy of the approximating polynomial was considered by Box and Draper (3, 4). They proposed the minimization of the mean squared error integrated over R as a basic criterion. This criterion considers bias and variance simultaneously. Consideration of bias seems pertinent in cases where a first order model is used; since the question arises as to whether or not the choice of a design can offer proper protection against the possibility of curvature in the true response surface. In the case of a second order design, one might be interested in a design which affords protection against the existence of cubic terms in the true response function.

Suppose an experimenter fits a polynomial model of order d_1 in the region of interest, R; however, the true model is a polynomial response of order d_2, where $d_2 \geq d_1$. The mean squared error integrated over R is

$$J = \frac{N\Omega}{\sigma^2} \int_R E(\hat{y}(\underset{\sim}{x}) - \eta(\underset{\sim}{x}))^2 d\underset{\sim}{x}$$

where $\Omega^{-1} = \int_R d\underset{\sim}{x}$ and σ^2 is the experimental error variance. The experimental errors are assumed to be independent and identically distributed with variance σ^2. It can be readily shown that

$$J = V + B$$

where

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

and

$$B = \frac{N\Omega}{\sigma^2} \int_R [E(\hat{y}(\underline{x})) - \eta(\underline{x})]^2 d\underline{x} \ .$$

Thus J is the sum of B, integrated squared bias, and V, integrated $\mathrm{Var}(y(\underline{x}))$.

Estimation requires calculation of the regression coefficients from experimental data. Box and Draper used the standard least squares method. Since the mean squared error criterion was introduced many researchers have concentrated on experimental design criteria which include bias as a consideration. Several authors (2, 10, 11, 12) have suggested different estimators for the regression coefficients to achieve smaller mean squared error under some circumstances.

All of these works regarding design criteria, whether they are variance oriented or bias oriented, have one thing in common, namely that they concern the estimation of the height of the response in the factor space rather than the estimation of differences in response. However, the main stream in statistical work on the design of experiments has been on the comparison of treatments, i.e., on the estimation of treatment contrasts. In this point of view the study of response surface designs has been exceptional since it has mainly emphasized the estimation of absolute response. This can be a serious oversight. Estimation of differences in response at different points in the factor space will often be of great importance. If differences at points close together are involved, estimation of the local slopes (the rates of change) of the response surface is of interest. This problem, estimation of slopes, occurs frequently in practical situations. For instance, there are the cases in which we want to estimate rates of reaction in chemical experiments, rates of change in the response of a plant to various fertilizers, rates of disintegration of radioactive material in an animal, etc.

The problem considered in this thesis is, therefore, that of the choice of the experimental design so as to achieve maximum information on the estimated slopes of the response surface. In designing these experiments allowance is made for bias, due to an inadequate model. The mean squared error of the estimated slope integrated over R will be the basic measure of information provided by the design. Only the least squares estimator of the slope will be considered.

This problem of estimating slopes is relatively unexplored in the literature. Several authors have considered the topic, but with limited discussions. Atkinson (1) mainly considers first order polynomials when the true models are quadratic. Ott and Mendenhall (15) discuss a second order polynomial, but they limit the case to a single variable and to a quadratic polynomial as a true response. Matteson (13) and Munsch (14) extend the concept of minimum bias estimation which was initially suggested by Karson, Manson and Hader (11) to the estimated slope of response surfaces.

In what follows we will pursue a thorough investigation of the topic in cases where second order polynomials are fitted for single and for several independent variables when the true responses are either quadratic or cubic. A new design concept called slope-rotatability will be introduced. Designs with points equally spaced on one, two or three circles will be investigated extensively. A computer search routine will be used to find optimum designs in this class.

2. ONE FACTOR EXPERIMENTAL DESIGNS

Suppose the true model is a polynomial of degree d_2 ,

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

in a single variable but for one reason or another the experimenter fits a polynomial of degree $d_1 \le d_2$,

$$\hat{y}(x) = \underline{x}_1'\underline{b}_1 ,$$

where $\underline{b}_1$ is the least squares estimate of $\underline{\beta}_1$. The mean squared error integrated over R for the estimated slope, $d\hat{y}/dx$, is

$$J = \frac{N\Omega}{\sigma^2}\int_R E\left(\frac{d\hat{y}}{dx} - \frac{d\eta}{dx}\right)^2 dx \qquad \text{where} \quad \Omega^{-1} = \int_R dx$$

$$= \frac{N\Omega}{\sigma^2}\int_R E\left[\frac{d\hat{y}}{dx} - E\left(\frac{d\hat{y}}{dx}\right)\right]^2 dx + \frac{N\Omega}{\sigma^2}\int_R \left[E\left(\frac{d\hat{y}}{dx}\right) - \frac{d\eta}{dx}\right]^2 dx$$

$$= V + B .$$

Thus J which we want to minimize as the design optimality criterion is the sum of integrated variance, denoted by V , and integrated squared bias, denoted by B .

In order that the bias portion can be evaluated the bias of the polynomial coefficients must first be evaluated. Suppose X_i is a matrix the elements of the $i^{\underline{th}}$ row of which are the values taken by the terms of $\underline{x}_i$ for the $i^{\underline{th}}$ experimental combination. The least squares estimator for $\underline{b}_1$ is

$$\underline{b}_1 = (X_1'X_1)^{-1}X_1'\underline{y}$$

where $\underline{y}$ is the vector of the N observations. Then the bias of the coefficients is given by

$$E(\underline{b}_1) - \underline{\beta}_1 = A\underline{\beta}_2$$

where A is $(X_1'X_1)^{-1}X_1'X_2$. The extent of the bias is determined by the matrix A , the alias matrix.

Designs for one variable are the subject of the following sections. In Section 2.1, designs for the linear model protecting against quadratic effect will be briefly discussed, and then in Sections 2.2 and 2.3 designs for the quadratic model when the true model is either quadratic or cubic will be investigated. The region of interest, R , is assumed to be $-1 \leq x \leq 1$.

2.1 Designs for the Linear Model When the True Response is Quadratic

If the true model is quadratic, $\eta(x) = \beta_0 + \beta_1 x + \beta_2 x^2$, and the first order model, $\hat{y}(x) = b_0 + b_1 x$, is fitted, how should experiments be designed so that the estimate of the slope is as precise as possible? Suppose the experiment consists of observations at two fixed factor levels. Atkinson (1) indicates that J is minimized when the observations are equally divided between the two equally spaced levels from the center of the design. We will only, therefore, discuss the designs with the trials equally divided between the two equally spaced factor levels from the design center. Our emphasis is on determining an "optimal" straight line fit with a small number of observations rather than on detecting departures from linearity. For the latter purpose more than two distinct levels would be needed.

Suppose N (even number) trials are allocated with N/2 trials on each -h level and h level where h is the distance from the center of the design. Then one can show that

$$V = \frac{N\Omega}{\sigma^2}\int_R E\left(\frac{d\hat{y}}{dx} - E\left(\frac{d\hat{y}}{dx}\right)\right)^2 dx \qquad \text{where} \quad \Omega^{-1} = \int_{-1}^{1} dx$$

$$= \frac{N}{2\sigma^2}\int_{-1}^{1} E(b_1 - \beta_1)^2 dx$$

since

$$E\left(\frac{d\hat{y}}{dx}\right) = E(b_1) = \beta_1 .$$

Then

$$V = \frac{N}{2\sigma^2}\int_{-1}^{1} \mathrm{Var}(b_1) dx$$

$$= \frac{N}{2\sigma^2}\int_{-1}^{1} \frac{\sigma^2}{Nh^2} dx$$

$$= \frac{1}{h^2} ,$$

and

$$B = \frac{N\Omega}{\sigma^2}\int_R \left(E\left(\frac{d\hat{y}}{dx}\right) - \frac{d\eta}{dx}\right)^2 dx$$

$$= \frac{N}{2\sigma^2}\int_{-1}^{1} (\beta_1 - (\beta_1 + 2\beta_2 x))^2 dx = \frac{N}{2\sigma^2}\int_{-1}^{1} (-2\beta_2 x)^2 dx$$

$$= \frac{4}{3}\left(\frac{\sqrt{N}\,\beta_2}{\sigma}\right)^2 .$$

Consequently, the mean squared error integrated over R is

$$J = V + B$$

$$= 1/h^2 + 4\alpha^2/3$$

where

$$\alpha = \frac{\sqrt{N}\,\beta_2}{\sigma} .$$

Observe that the bias, $-2\beta_2 x$, is zero only at the center of R and the squared bias, B, is independent of h. Also the integrated variance, V, is a monotonically decreasing function of h. J is thus minimized for any given α when h takes on the largest feasible value.

The region of operability could be larger than R; however, in nearly all practical problems there is obviously some practical limit or bound on h. If h is assumed to be bounded by b, then J is minimized at $h = b$. Atkinson (1) discusses this case extensively generalizing R to be the line of length $2c$ centered at an arbitrary point x_0. Atkinson assumes that the region of operability is $-1 \le x \le 1$.

2.2 Designs for the Quadratic Model When the True Model is Also Quadratic

If the fitted model happens to be the true model, bias is zero. In this case J is equal to V and the design criterion is simply to minimize the integrated variance of the estimated slope over R.

The estimation of the slope of the second order model requires a minimum of three levels of the independent variable since there are three parameters in the model, $\hat{y} = b_0 + b_1x + b_2x^2$. It is shown by de la Garza (7) that the precision matrix (variance-covariance matrix) of least squares estimators in the model for a design at more than three levels of the variable can always be obtained by spacing at just three judiciously selected levels of the variable. Therefore, in what follows in this section the selection of three levels of the variable and the allocation of N trials ot the three levels, equally spaced with the center level at zero, will be considered.

Suppose N trials are allocated as below:

$-h$	0	h	
n_1	n_0	n_1	trials

The same number of trials are allocated to both extreme levels since one can show that the design criterion is minimized when the both levels have an equal number of trials. For the above allocation scheme the design matrix is

$$
X = \begin{array}{c}
\begin{array}{ccc} & x & x^2 \end{array} \\
\left[\begin{array}{ccc}
1 & -h & h^2 \\
1 & -h & h^2 \\
\vdots & \vdots & \vdots \\
1 & -h & h^2 \\
1 & 0 & 0 \\
1 & 0 & 0 \\
\vdots & \vdots & \vdots \\
1 & 0 & 0 \\
1 & h & h^2 \\
1 & h & h^2 \\
\vdots & \vdots & \vdots \\
1 & h & h^2
\end{array}\right]
\end{array}
\begin{array}{l}
\\
\\
\cdots \quad n_1 \text{ trials} \\
\\
\\
\\
\cdots \quad n_0 \text{ trials} \\
\\
\\
\\
\cdots \quad n_1 \text{ trials} \\
\\
\end{array}
$$

Note that X is used instead of X_1 since there is no X_2 matrix involved in this section. One can easily obtain

$$(X'X)^{-1} = \begin{bmatrix} \frac{1}{N-2n_1} & 0 & \frac{-1}{h^2(N-2n_1)} \\ 0 & \frac{1}{2n_1h^2} & 0 \\ \frac{-1}{h^2(N-2n_1)} & 0 & \frac{N}{2n_1h^4(N-2n_1)} \end{bmatrix} .$$

From the model, $\hat{y} = b_0 + b_1x + b_2x^2$, the estimated slope at x is $d\hat{y}/dx = b_1 + 2b_2x$. Thus its variance is

$$V^* = \mathrm{Var}(d\hat{y}/dx)$$

$$= \mathrm{Var}(b_1 + 2b_2x)$$

$$= \left[\frac{1}{2n_1h^2} + 4x^2\left(\frac{N}{2n_1h^4(N-2n_1)}\right)\right]\sigma^2 .$$

The integrated variance over R is

$$V = \frac{N\Omega}{\sigma^2}\int_R V^*\,dx \qquad \text{where} \quad \Omega^{-1} = \int_{-1}^{1} dx$$

$$= \frac{N}{2n_1h^2} + \frac{2N^2}{3n_1h^4(N-2n_1)} . \qquad (2)$$

Letting $f = n_1/N$, we can write the integrated variance as

$$V = \frac{1}{2h^2f} + \frac{2}{3h^4f(1-2f)} . \qquad (3)$$

Equation (3) indicates that to minimize V, h should be as large as feasible within the region of operability. Once h is fixed, the minimizing value of f , f* , can be obtained by solving $dV/df = 0$, which is

$$f^* = \frac{3h^2+4) - 2\sqrt{3h^2+4}}{6h^2} .$$

For various choices of h , Table 1 shows the corresponding f* and V_{min} , the minimum value of V . Table 1 provides an interesting aspect that f* stays within a narrow range as h changes over a quite wide range. Note that for $h = 1$, f* is equal to 0.2847 which agrees with Atkinson's result. In practice, since n_1 is an integer, the optimum f* can only be approximately achieved unless a large number of trials are observed.

Another aspect which should be pointed out is that even though f* is a fairly narrow interval for different values of h , nevertheless the integrated variance is not terribly sensitive to f for a given h . For example, with $h = 1$, $f^* = 0.2847$ with $V_{min} = 7.195$; however, if $f = 0.25$, $V = 7.333$. Therefore, 25% allocation of the trials at an extreme level instead of 28.47% is quite acceptable as a good design. Incidently, Ott and Mendenhall (15) recommended 25% allocation to an extreme level based on their criterion, the minimization of the rate of curvature of $N\ Var(d\hat{y}/dx)/\sigma^2$.

Table 1 f^* and V_{min} for fixed h

h	f*	V_{min}
0.7	0.2695	26.135
0.8	0.2744	15.993
0.9	0.2795	10.452
1.0	0.2847	7.195
1.1	0.2900	5.163
1.2	0.2953	3.835
1.3	0.3005	2.931
1.4	0.3056	2.295
1.5	0.3106	1.835

2.3 Designs for the Quadratic Model When the True Model is Cubic

In this section we will discuss second order designs which can afford protection against the existence of a cubic term in the true response function,

$$\eta(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 .$$

The class of designs to be considered is the same class we studied in Section 2.2, that is, designs with three equally spaced levels, $-h$, 0 and h, of the independent variable and allocation of trials, n_1, n_0 and n_1, respectively, on each level. For this class of designs X_1 is identical to X in the previous section and X_2 is given by

$$X_2' = (\underbrace{-h^3, -h^3, \ldots, -h^3}_{n_1 \text{ trials}} \ \underbrace{0, 0, \ldots, 0}_{n_0 \text{ trials}} \ \underbrace{h^3, h^3, \ldots, h^3}_{n_1 \text{ trials}}) .$$

The precision matrix, $(X_1'X_1)^{-1}$, is equal to $(X'X)^{-1}$ in the previous section, and

$$X_1'X_2 = \begin{bmatrix} 0 \\ 2n_1h^4 \\ 0 \end{bmatrix} .$$

Hence, the alias matrix is

$$A = (X_1'X_1)^{-1}X_1'X_2 = \begin{bmatrix} 0 \\ h^2 \\ 0 \end{bmatrix} .$$

Here, the vector $\underline{\beta}_2$ takes the form of the single element β_3. Thus we can obtain

$$E(\underline{b}_1) = E\begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \underline{\beta}_1 + A\underline{\beta}_2 = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} 0 \\ h^2 \\ 0 \end{bmatrix} \beta_3$$

$$= \begin{bmatrix} \beta_0 \\ \beta_1 + h^2\beta_3 \\ \beta_2 \end{bmatrix} .$$

Consequently, the bias of the estimated slope at a point x is

$$E(d\hat{y}/dx) - \frac{d\eta}{dx} = E(b_1 + 2b_2x) - (\beta_1 + 2\beta_2x + 3\beta_3x^2)$$

$$= (\beta_1 + h^2\beta_3 + 2\beta_2x) - (\beta_1 + 2\beta_2x + 3\beta_3x^2)$$

$$= h^2\beta_3 - 3\beta_3x^2 ,$$

and the integrated squared bias over R is

$$B = \frac{N\Omega}{\sigma^2}\int_R [E(\frac{d\hat{y}}{dx}) - \frac{d\eta}{dx}]^2 \qquad \text{where} \quad \Omega^{-1} = \int_{-1}^{1} dx$$

$$= \frac{N}{2\sigma^2}\int_{-1}^{1} (h^2\beta_3 - 3\beta_3 x^2)^2 dx$$

$$= \alpha^2(h^4 - 2h^2 + 1.8) \qquad \text{where} \quad \alpha = \frac{\sqrt{N}\,\beta_3}{\sigma} . \tag{4}$$

Note that B is independent of $f = n_1/N$ and achieves minimum at $h = 1$. Since the integrated variance, V, is the same as that in Section 2.2, the mean squared error over R is

$$J = V + B$$

$$= [\frac{1}{2fh^2} + \frac{2}{3fh^4(1-2f)}] + \alpha^2(h^4 - 2h^2 + 1.8) . \tag{5}$$

Since B is minimized at $h = 1$ and V is a monotonically decreasing function of h, J will be minimized at $1 \leq h < +\infty$ for any given α. For a fixed value of h one can find the minimizing value of f, f^*, by setting

$$dJ/df = 0$$

which implies

$$f^* = \frac{(3h^2 + 4) - 2\sqrt{3h^2 + 4}}{6h^2} .$$

This is the same equation for f^* as appeared in the previous section, simply because B is independent of f and V has the same

Table 2 h^* and f^* for given α

α	h^*	f^*	V	B	J (Optimum)	J (when h is limited to R)
0	$\to +\infty$		$\to 0$	0	$\to 0$	7.195
1	1.397	0.3054	2.311	1.706	4.017	7.995
2	1.225	0.2966	3.577	4.202	7.779	10.395
3	1.150	0.2926	4.432	8.136	12.568	14.395
4	1.104	0.2902	5.099	13.566	18.665	19.995
$+\infty$	1.000	0.2847	7.195	$+\infty$	$+\infty$	$+\infty$

form as before. If h is limited to R, $-1 \le x \le 1$, the h which minimizes J (call this h^*) is 1 and $f^* = 0.2847$ for any given α.

Table 2 is constructed to show how h^* and f^* depend on α. The h^* and f^* are obtained by trial-and-error, and were checked by substitution into the equation found by setting $\partial J/\partial f = 0$ and $\partial J/\partial h = 0$. The last column in Table 2 shows the values of J when h is limited to R, that is, when $h^* = 1$ and $f^* = 0.2847$.

Several aspects can be observed from Table 2. As α increases, h^* decreases approaching 1 and f^* also decreases approaching 0.2847. The range of h^* as α changes is quite wide, however, f^* stays within a narrow range.

3. MULTIFACTOR EXPERIMENTAL DESIGNS

The slope of the response surface for a single variable at any point is a scalar. However, with more than one variable the slope depends on the direction of measurement. In this chapter the general method of estimation of slope for p variables will first be developed and then the criterion of rotatability for the variance of estimated slope will be extensively discussed.

Suppose the d_1 order polynomial model, $\hat{y}(\underline{x}) = \underline{x}_1'\underline{b}_1$, is fitted protecting against the bias effect, if any, of the d_2 order polynomial model, $\eta(\underline{x}) = \underline{x}_1'\underline{\beta}_1 + \underline{x}_2'\underline{\beta}_2$. Let X_i be a matrix, the elements of the $i^{\underline{th}}$ row of which are the values taken by the terms of $\underline{x}_i$ for the $i^{\underline{th}}$ experimental combination. Also let

$$\underline{g}(\underline{x}) = \begin{pmatrix} \frac{\partial \hat{y}}{\partial x_1} \\ \frac{\partial \hat{y}}{\partial x_2} \\ \vdots \\ \frac{\partial \hat{y}}{\partial x_p} \end{pmatrix} = D_1\underline{b}_1 \quad \text{and} \quad \underline{r}(\underline{x}) = \begin{pmatrix} \frac{\partial \eta}{\partial x_1} \\ \frac{\partial \eta}{\partial x_2} \\ \vdots \\ \frac{\partial \eta}{\partial x_p} \end{pmatrix} = D_1\underline{\beta}_1 + D_2\underline{\beta}_2$$

where D_j is a matrix, the $i^{\underline{th}}$ row of which is obtained by the parital differentiation of $\underline{x}_j'$ with respect to x_i . The elements of $\underline{g}(\underline{x})$ are the estimates of the slope of the fitted response surface and the elements of $\underline{r}(\underline{x})$ are those of the true response surface along the p factor axes. Therefore, the slope at $\underline{x}$ on the fitted response surface in the direction specified by the $p \times 1$ vector of direction cosines, $\underline{k}' = (k_1, k_2, k_3, \ldots, k_p)$, is a linear combination of $\underline{g}$, that is $\underline{k}'\underline{g}$. If we let $\underline{s} = E(\underline{g}) - \underline{r}$, then $\underline{s}$ represents the vector of biases of the estimated slopes along the p factor axes estimated at the point $\underline{x}$.

The mean squared error of the estimated slope in a specified direction $\underline{k}$ at a point $\underline{x}$ is

$$J^* = E(\underline{k}'\underline{g} - \underline{k}'\underline{r})^2$$

$$= \mathrm{Var}(\underline{k}'\underline{g}) + (E(\underline{k}'\underline{g}) - \underline{k}'\underline{r})^2$$

$$= \underline{k}'\mathrm{Var}(\underline{g})\underline{k} + (\underline{k}'\underline{s})'(\underline{k}'\underline{s})$$

$$= \underline{k}'D_1\mathrm{Var}(\underline{b}_1)D_1'\underline{k} + \underline{s}'\underline{kk}'\underline{s} \tag{6}$$

$$= V^* + B^*$$

where $V^* = \underline{k}'D_1\mathrm{Var}(\underline{b}_1)D_1'\underline{k}$ is the variance component and $B^* = \underline{s}'\underline{kk}'\underline{s}$ is the squared bias component. If $\underline{k}$ were known, experiments would be designed to minimize equation (6). If the direction of interest, $\underline{k}$, is not specified in advance, one might wish to average J^* over all directions in such a way that the distribution over all directions is uniform. The following lemmas will enable us to average J^* over all directions.

<u>Lemma 1</u>: The average of V^* over all directions is

$$\bar{V}^* = \frac{\sigma^2}{p}\,\mathrm{tr}(D_1(X_1'X_1)^{-1}D_1') \,. \tag{7}$$

Proof: Let $M = D_1 \mathrm{Var}(\underline{b}_1) D_1'$. The average of V^* over all directions in such a way that the distribution over all directions is uniform is

$$\bar{V}^* = \underset{\underline{k}}{\mathrm{Average}}(\underline{k}'M\underline{k})$$

$$= \underset{\underline{k}}{\mathrm{Average}}[\mathrm{tr}(\underline{k}'M\underline{k})] \quad \text{since } \underline{k}'M\underline{k} \text{ is a scalar,}$$

$$= \underset{\underline{k}}{\mathrm{Average}}[\mathrm{tr}(M\underline{k}\underline{k}')]$$

$$= \mathrm{tr}[\underset{\underline{k}}{\mathrm{Average}}(M\underline{k}\underline{k}')]$$

$$= \mathrm{tr}[M(\underset{\underline{k}}{\mathrm{Average}}(\underline{k}\underline{k}'))] .$$

Therefore, we have to calculate

$$\underset{\underline{k}}{\mathrm{Average}}(\underline{k}\underline{k}') = C\int \underline{k}\underline{k}' dA$$

where C is a proper average constant and dA is the area element of the hypersphere with unit radius.

It can be shown (Appendix 7.9) that $C\int \underline{k}\underline{k}' dA$ is a diagonal matrix whose diagonal elements are all equal. Let $C\int \underline{k}\underline{k}'\, dA = vI_p$, then

$$\bar{V}^* = \mathrm{tr}(MvI_p)$$

$$= \mathrm{tr}(vM)$$

$$= v\,tr(M)$$

$$= v \sum_{i=1}^{p} \lambda_i$$

where λ_i's are eigenvalues of M. Notice that v is independent of M and is only associated with $C\int \underline{k}\underline{k}'dA$. To find the constant v suppose M is the identity matrix. The average of $\underline{k}'M\underline{k}$ is 1 and $\lambda_i = 1$ for all i. Therefore, $v = 1/p$ and $\bar{\bar{V}}^*$ becomes

$$\bar{\bar{V}}^* = (1/p)tr(M)$$

$$= (1/p)tr(D_1 Var(\underline{b}_1)D_1')$$

$$= \frac{\sigma^2}{p}\, tr(D_1(X_1'X_1)^{-1}D_1') \quad \text{since} \quad Var(\underline{b}_1) = (X_1'X_1)^{-1}\sigma^2 .$$

Q. E. D.

Lemma 2: The average of B^* over all directions is

$$\bar{\bar{B}}^* = (1/p)\underline{s}'\underline{s} . \tag{8}$$

Proof:

$$\bar{\bar{B}}^* = \text{Average } (\underline{s}'\underline{k}\underline{k}'\underline{s})$$

$$= C\int \underline{s}'\underline{k}\underline{k}'\underline{s}dA$$

$$= \underline{s}'[C\int \underline{k}\underline{k}'dA]\underline{s} \quad \text{since } \underline{s} \text{ is independent of } \underline{k} ,$$

$$= v\underline{s}'\underline{s}$$

$$= (1/p)\underline{s}'\underline{s} \ .$$

Q. E. D.

The relation, $v = 1/p$, can be verified differently in the following way in Lemma 2. Suppose $\underline{s}' = (1, 1, \ldots, 1)$. Then $\underline{s}'\underline{s} = p$ and $\bar{B}^* = 1$. Hence, $v = 1/p$ from $\bar{B}^* = v\underline{s}'\underline{s}$. From Lemmas 1 and 2 it is immediately obtained that the average J^* over all directions is

$$\bar{J}^* = \bar{V}^* + \bar{B}^*$$

$$= \frac{\sigma^2}{p} \operatorname{tr}(D_1(X_1'X_1)^{-1}D_1') + (1/p)\underline{s}'\underline{s} \ . \tag{9}$$

If we do not specify the point of interest at which the slope is to be estimated, experiments should be designed to minimize the mean squared error integrated over the region of interest, R . The mean squared error integrated over R is

$$J = \frac{N\Omega}{\sigma^2} \int_R \bar{J}^* \, d\underline{x} \qquad \text{where} \qquad \Omega^{-1} = \int_R d\underline{x}$$

$$= \frac{N\Omega}{\sigma^2} \int_R (\bar{V}^* + \bar{B}^*) d\underline{x}$$

$$= V + B$$

$$= \frac{N}{p} \operatorname{tr}[(X_1'X_1)^{-1}W_{11}]$$

$$+ \frac{N}{p\sigma^2} \operatorname{tr}[\underline{\beta}_2\underline{\beta}_2'(A'W_{11}A - 2A'W_{12} + W_{22})] \tag{10}$$

where

$$A = (X_1'X_1)^{-1}X_1'X_2$$

$$W_{11} = \Omega\int_R D_1'D_1 d\underline{x}$$

$$W_{12} = \Omega\int_R D_1'D_2 d\underline{x}$$

$$W_{22} = \Omega\int_R D_2'D_2 d\underline{x} \ .$$

The derivation of equation (10) is obtained in the following way: The integrated variance is

$$V = \frac{N\Omega}{\sigma^2}\int_R \bar{V}^* d\underline{x}$$

$$= \frac{N\Omega}{\sigma^2}\int_R \frac{\sigma^2}{p}\, tr(D_1(X_1'X_1)^{-1}D_1')d\underline{x}$$

$$= \frac{N\Omega}{p}\int_R tr((X_1'X_1)^{-1}D_1'D_1)d\underline{x}$$

$$= \frac{N}{p}\, tr((X_1'X_1)^{-1}W_{11}) \tag{11}$$

and the integrated squared bias is

$$B = \frac{N\Omega}{\sigma^2}\int_R \bar{B}^* d\underline{x}$$

$$= \frac{N\Omega}{\sigma^2}\int_R \frac{1}{p}\,\underline{s}'\underline{s}d\underline{x}$$

$$= \frac{N\Omega}{p\sigma^2}\int_R [(D_1A - D_2)\underline{\beta}_2]'[(D_1A - D_2)\underline{\beta}_2]d\underline{x}$$

since

$$\underline{s} = E(\underline{g}) - \underline{r}$$

$$= D_1 E(\underline{b}_1) - (D_1\underline{\beta}_1 + D_2\underline{\beta}_2)$$

$$= D_1(\underline{\beta}_1 + (X_1'X_1)^{-1}X_1'X_2\underline{\beta}_2) - (D_1\underline{\beta}_1 + D_2\underline{\beta}_2)$$

$$= D_1A\underline{\beta}_2 - D_2\underline{\beta}_2$$

$$= (D_1A - D_2)\underline{\beta}_2 \ . \tag{12}$$

So

$$B = \frac{N\Omega}{p\sigma^2} \int_R \underline{\beta}_2'(A'D_1' - D_2')(D_1A - D_2)\underline{\beta}_2 d\underline{x}$$

$$= \frac{N\Omega}{p\sigma^2} \int_R tr(\underline{\beta}_2'(A'D_1'D_1A - A'D_1'D_2 - D_2'D_1A + D_2'D_2)\underline{\beta}_2)d\underline{x}$$

$$= \frac{N}{p\sigma^2} tr[\underline{\beta}_2\underline{\beta}_2'(A'W_{11}A - 2A'W_{12} + W_{22})] \ . \tag{13}$$

For the case when the first order model is fitted when the true model is quadratic, a comprehensive study can be found in the paper by Atkinson (1). Accordingly, we will only consider the cases where the second order polynomial models are fitted.

3.1 Designs for the Quadratic Model When the True Model is Also Quadratic

If we fit the quadratic model when the true model is also quadratic, there is no bias involved and the variance of the estimated slope is the only concern. The quadratic model with p variables, $\hat{y}(\underline{x}) = \underline{x}_1'\underline{b}_1$, will have

$$\underline{x}_1' = (1, x_1, x_2, \ldots, x_p; x_1^2, x_2^2, \ldots, x_p^2; x_1x_2, x_1x_3, \ldots, x_{p-1}x_p)$$

and

$$\underline{b}_1' = (b_0, b_1, b_2, \ldots, b_p; b_{11}, b_{22}, \ldots, b_{pp}; b_{12}, b_{13}, \ldots, b_{p-1,p}) .$$

In this section X, D, $\underline{x}$ and $\underline{b}$ will be used instead of X_1, D_1, $\underline{x}_1$ and $\underline{b}_1$ for notational convenience since X_2, D_2, $\underline{x}_2$ and $\underline{b}_2$ are not needed. Notice that $\underline{s} = E(\underline{g}) - \underline{r} = \underline{0}$.

As we have obtained before, the average variance of the estimated slopes at $\underline{x} = (x_1, x_2, \ldots, x_p)$ over all directions is

$$\bar{V}^* = \frac{\sigma^2}{p} \operatorname{tr}(D(X'X)^{-1}D')$$

which is a function of the coordinates of the point, $\underline{x}$, as well as of the design used and also, of course, of σ^2. $\bar{V}^*$ can be reduced by increasing N. The quantity, $V(\underline{x}) = N\bar{V}^*/\sigma^2$, is thus a standardized measure of precision of estimation. $V(\underline{x})$ will be called the variance function of the design. In other words, for any experimental design $V(\underline{x})$ provides a standardized measure of the precision of the estimated slopes averaged over all directions at the point $\underline{x}$ in the space of the variables. It is a function of $\underline{x}$ and the elements of the precision matrix, $(X'X)^{-1}$, and is uniquely defined for every p-dimensional experimental design.

Suppose we have two points which are equidistant from the design center. If there is a considerable difference between the two points as far as precision of the estimated slopes is concerned, a certain "imbalance" exists in the use of the surface. Therefore, in the study of response surface design an important and interesting property is that of rotatability due to Box and Hunter (5). As mentioned in Chapter 1, for a rotatable design $Var(\hat{y})$ will be the same for any two points which are the same distance from the design center. This concept of rotatability is now introduced here with respect to the variance function, $V(\underline{x})$, for the slope estimate. Suppose $V(\underline{x})$ for a p-dimensional design is a function only of

$$\rho = \sum_{i=1}^{p} x_i^2 ,$$

the distance from the center, so that the variance function contours in the space of the variables are circles, spheres or hyperspheres centered at the origin. A design giving such a variance function will be called a slope-rotatable design and rotatability in the Box-Hunter sense will henceforth be called $\hat{y}$-rotatability.

3.1.1 Properties of Slope-Rotatability

As a first step to develop slope-rotatable designs, we propose a theorem giving the conditions for slope-rotatability. The notation (i,j) will mean a combination of i and j .

<u>Theorem 1</u>: The necessary and sufficient conditions that a design be slope-rotatable are that

1) $$2Cov(b_i, b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} Cov(b_j, b_{ij}) = 0 \quad \text{for all } i ,$$

2) $$2(Cov(b_{ii}, b_{ij}) + Cov(b_{jj}, b_{ij})) + \sum_{\substack{k=1 \\ k\neq i,j}}^{p} Cov(b_{ik}, b_{jk}) = 0$$

for any (i,j) where $i \neq j$.

3) $4\text{Var}(b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} \text{Var}(b_{ij})$ are equal for all i .

Proof: It can be shown that

$$\bar{V}^* = \frac{\sigma^2}{p} \text{tr}(D(X'X)^{-1}D')$$

$$= \frac{1}{p} \text{tr}((X'X)^{-1}\sigma^2 D'D)$$

$$= \frac{1}{p} \sum_{i=1}^{p} \text{Var}(b_i) + \frac{2}{p} \sum_{i=1}^{p} x_i(2\text{Cov}(b_i, b_{ii})$$

$$+ \sum_{\substack{j=1 \\ j\neq i}}^{p} \text{Cov}(b_j, b_{ij}))$$

$$+ \frac{2}{p} \sum_{\substack{(i,j) \\ i\neq j}}^{p} x_i x_j [2(\text{Cov}(b_{ii}, b_{ij}) + \text{Cov}(b_{jj}, b_{ij}))$$

$$+ \sum_{\substack{k=1 \\ k\neq i,j}}^{p} \text{Cov}(b_{ik}, b_{jk})]$$

$$+ \frac{1}{p} \sum_{i=1}^{p} x_i^2 [4\text{Var}(b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} \text{Var}(b_{ij})] \; . \tag{14}$$

Note that the conditions in the theorem are sufficient for equation (14) to be a function only of the distance from the center. If these conditions are satisfied, then $\bar{V}^*$ can be written as

$$\bar{V}^* = \frac{1}{p}\sum_{i=1}^{p} \mathrm{Var}(b_i) + \frac{1}{p}[4\,\mathrm{Var}(b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} \mathrm{Var}(b_{ij})]\sum_{i=1}^{p} x_i^2 \quad (15)$$

which is only a function of

$$\rho = \sum_{i=1}^{p} x_i^2 .$$

Suppose at least one of the three conditions are not satisfied. Then it is easy to show that there exist two points which are the same distance from the design center, but which give different values of $\bar{V}^*$. Therefore, the conditions are also necessary. Q. E. D.

The three corollaries immediately following are based on the theorem. They are useful in constructing slope-rotatable designs.

Corollary 1: All $\hat{y}$-rotatable designs are slope-rotatable.

Proof: Box and Hunter (5) show that the covariances associated with conditions 1 and 2 in theorem 1 are all zero for $\hat{y}$-rotatable designs, and, furthermore, $\mathrm{Var}(b_{ii})$ are equal for all i and $\mathrm{Var}(b_{ij})$ are also equal for all (i,j) where $i \neq j$. Therefore, conditions 1, 2 and 3 are obviously satisfied for $\hat{y}$-rotatable designs. Thus, they are slope-rotatable. Q. E. D.

Corollary 2: If all odd moments are zero, then only condition 3 is necessary and sufficient for slope-rotatability.

Proof: If all odd moments are zero, then the covariances in conditions 1 and 2 are all zero, which implies that the two conditions are satisfied. The only remaining condition is 3. Q. E. D.

Corollary 3: If all odd moments are zero and all mixed fourth mements are equal, that is

$$[i^2 j^2] = \frac{1}{N} \sum_{k=1}^{N} x_{ik}^2 x_{jk}^2$$

are equal for all (i,j) , $i \neq j$, then the necessary and sufficient condition for slope-rotatability is: Equal $\mathrm{Var}(b_{ii})$ for all i .

Proof: If all odd moments are zero, then only condition 3 is necessary and sufficient from Corollary 2. If all mixed fourth moments are equal, then it can be shown that $\mathrm{Var}(b_{ij})$ are equal for all (i,j) , $i \neq j$. Therefore, the condition that $\mathrm{Var}(b_{ii})$ are equal for all i is the only remaining necessary and sufficient condition. Q. E. D.

If $p = 2$ Corollary 3 is particularly useful, since then there is only one mixed fourth moment, $[1^2 2^2]$, which implies that all mixed fourth moments are always equal. To make the theorem and its three corollaries more concrete, the two independent variables case will be considered in detail.

For the case of $p = 2$, $\underline{x}$, $\underline{b}$, X , and D take the following forms:

$$\underline{x}' = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2) ,$$

$$\underline{b}' = (b_0, b_1, b_2, b_{11}, b_{22}, b_{12}) ,$$

$$X = \begin{bmatrix} 1 & x_{11} & x_{21} & x_{11}^2 & x_{21}^2 & x_{11}x_{21} \\ 1 & x_{12} & x_{22} & x_{12}^2 & x_{22}^2 & x_{12}x_{22} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1N} & x_{2N} & x_{1N}^2 & x_{2N}^2 & x_{1N}x_{2N} \end{bmatrix}$$

and

$$D = \begin{bmatrix} 0 & 1 & 0 & 2x_1 & 0 & x_2 \\ 0 & 1 & 0 & 0 & 2x_2 & x_1 \end{bmatrix} .$$

The variance function will be

$$V(\underline{x}) = \frac{N\bar{V}^*}{\sigma^2}$$

$$= \frac{N}{p} \operatorname{tr}(D(X'X)^{-1}D')$$

$$= \frac{N}{2\sigma^2} [\operatorname{Var}(b_1) + \operatorname{Var}(b_2) + 2x_1(2\operatorname{Cov}(b_1,b_{11})$$

$$+ \operatorname{Cov}(b_2,b_{12})) + 2x_2(2\operatorname{Cov}(b_2,b_{22})$$

$$+ \operatorname{Cov}(b_1,b_{12})) + x_1^2(4\operatorname{Var}(b_{11})$$

$$+ \operatorname{Var}(b_{12})) + x_2^2(4\operatorname{Var}(b_{22}) + \operatorname{Var}(b_{12}))$$

$$+ 4x_1x_2(\operatorname{Cov}(b_{11},b_{12}) + \operatorname{Cov}(b_{22},b_{12}))] .$$

To be slope-rotatable from Theorem 1, the following conditions should be satisfied.

$$2\mathrm{Cov}(b_1,b_{11}) + \mathrm{Cov}(b_2,b_{12}) = 0 \ ,$$

$$2\mathrm{Cov}(b_2,b_{22}) + \mathrm{Cov}(b_1,b_{12}) = 0 \ ,$$

$$\mathrm{Cov}(b_{11},b_{12}) + \mathrm{Cov}(b_{22},b_{12}) = 0 \ ,$$

and

$$4\mathrm{Var}(b_{11}) + \mathrm{Var}(b_{12}) = 4\mathrm{Var}(b_{22}) + \mathrm{Var}(b_{12}) \ .$$

Notice that the first two equalities come from condition 1 of Theorem 1, the third from condition 2 and the last from condition 3. The last condition above is, in fact, equal to $\mathrm{Var}(b_{11}) = \mathrm{Var}(b_{22})$ since $\mathrm{Var}(b_{12})$ cancels out. If the conditions hold, then the variance function becomes

$$V(\underline{x}) = \frac{N}{2\sigma^2}\left[\mathrm{Var}(b_1) + \mathrm{Var}(b_2) + (4\mathrm{Var}(b_{11}) + \mathrm{Var}(b_{12}))\rho^2\right] \tag{16}$$

where $\rho^2 = x_1^2 + x_2^2$. This function, $V(\underline{x})$, depends only on the distance, ρ , from the design center, that is, the variance contours are to be circles surrounding the design center.

For example, suppose the nine points of the 3^2 symmetric factorial design with three levels, -1, 0 and 1 for each variable were used. For this particular symmetric design, it is easy to show that all odd mements are zero, $\mathrm{Var}(b_1) = \mathrm{Var}(b_2) = \sigma^2/6$, $\mathrm{Var}(b_{11}) = \mathrm{Var}(b_{22}) =$

$= \sigma^2/2$ and $\mathrm{Var}(b_{12}) = \sigma^2/4$. From Corollary 2 or 3 this design is slope-rotatable. The variance function for the design is thus from equation (16)

$$V(\underline{x}) = \frac{N}{\sigma^2} \bar{V}^* = \frac{3}{2} + \frac{81}{8} \rho^2 . \tag{17}$$

The variance contours of equation (17) are shown in Figure 1.

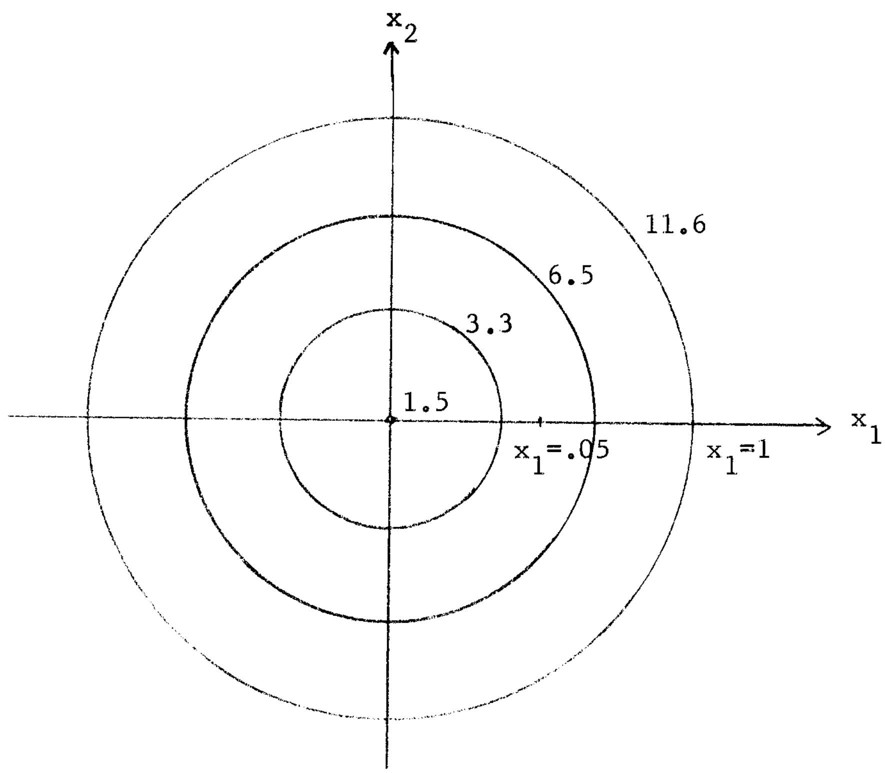


Figure 1 Variance contours for 3^2 factorial design

An interesting point is that this 3^2 factorial design is not $\hat{y}$-rotatable. From Corollary 1 we know that all $\hat{y}$-rotatable designs are slope-rotatable. However, the reverse is not true. The 3^2 factorial design is an example for the assertion. In fact, there are many more slope-rotatable designs which are not $\hat{y}$-rotatable. Such designs will appear in subsequent sections.

Another interesting point for a slope-rotatable design is that the variance function is a monotonically increasing function of ρ with a minimum at the design center. It is easy to prove this property. Consider equation (15). The coefficient of ρ^2,

$$\frac{1}{p}\left[4\mathrm{Var}(b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} \mathrm{Var}(b_{ij})\right],$$

is always positive, and consequently $dV(\underline{x})/dp > 0$ for a slope-rotatable design. Note that the variance function of a $\hat{y}$-rotatable design is not in general a monotonically increasing function.

If the point at which the slope is to be estimated could be anywhere within the region of interest, R, experiments should be designed to minimize $V(\underline{x})$ integrated over R. The integrated variance is then

$$V = \Omega\int_R V(\underline{x})d\underline{x} \qquad \text{where} \qquad \Omega^{-1} = \int_R d\underline{x}$$

$$= \Omega\int_R \frac{N}{\sigma^2}\bar{V}^* \, d\underline{x}$$

$$= \frac{N}{p}\,\mathrm{tr}((X'X)^{-1}W_{11})$$

as has been established in equation (11).

As mentioned earlier, with two or more independent variables the slope at a point $\underline{x}$ on the response surface depends on the direction of measurement. If the direction, $\underline{k}$, is not specified, experiments would be designed to minimize the average variance, $\bar{V}^*$, over all directions at point $\underline{x}$. Furthermore, if the point $\underline{x}$ is not specified, the experimenter would want to minimize the average $\bar{V}^*$ integrated over R. However, as Theorem 2 shows below, it will not be necessary, under some conditions, to average V^* over all directions to find $\bar{V}^*$, and subsequently V. There is a short-cut method to evaluate V directly from V^*. The region of interest, R, is assumed to be either the unit circle or the unit square centered at the origin of the design.

<u>Theorem 2</u>: If a design is slope-rotatable and $\mathrm{Var}(b_i)$ are equal for all i, then for the design

$$V = \frac{N\Omega}{\sigma^2} \int_R \bar{V}^* \, d\underline{x} = \frac{N\Omega}{\sigma^2} \int_R V_i^* d\underline{x}$$

for any i where V_i^* is the variance V^* of the estimated slope along the x_i factor axis.

<u>Proof</u>: We want to show that under the two conditions -- the design is slope-rotatable and has the same $\mathrm{Var}(b_i)$ -- $V = \frac{N\Omega}{\sigma^2} \int_R \bar{V}^* d\underline{x}$, the integrated $\bar{V}^*$ over R, is the same as the integrated V_i^* over R for any i where V_i^* is V^* along the x_i factor axis. From equation (6) for a specified direction $\underline{k}$,

$$V^* = \underline{k}'D\ \mathrm{Var}(\underline{b})D'\underline{k}$$

$$= \underline{k}'D(X'X)^{-1}D'\underline{k}\sigma^2 .$$

For the direction of the x_i factor axis, $\underline{k}$ is $\underline{k}' = (0,0,\ldots,1,\ldots,0)$ where 1 appears in the $i^{\underline{th}}$ place from the left and all remaining elements are zero. In this case it is easy to show that $\underline{k}'D = \underline{d}_i$, the $i^{\underline{th}}$ row of D matrix. Then

$$V_i^* = \underline{d}_i(X'X)^{-1}\underline{d}_i'\sigma^2 \ .$$

Now we want to show that

$$\int_R \bar{\bar{V}}^* d\underline{x} = \int_R V_i^* d\underline{x}$$

under the conditions. It can be shown that

$$V_i^* = \underline{d}_i(X'X)^{-1}d_i'\sigma^2$$

$$= \underline{d}_i[(X'X)^{-1}\sigma^2]\underline{d}_i'$$

$$= \mathrm{Var}(b_i) + 4\mathrm{Cov}(b_i, b_{ii})x_i + 2\sum_{\substack{j=1 \\ j\neq i}}^{p} \mathrm{Cov}(b_i, b_{ij})x_j$$

$$+ 4\sum_{\substack{j=1 \\ j\neq i}}^{p} x_i x_j \mathrm{Cov}(b_{ii}, b_{ij}) + 2\sum_{\substack{(k,\ell) \\ k,\ell\neq i \\ k\neq\ell}}^{p} \mathrm{Cov}(b_{ik}, b_{i\ell})x_k x_\ell$$

$$+ 4\mathrm{Var}(b_{ii})x_i^2 + \sum_{\substack{j=1 \\ j\neq i}}^{p} \mathrm{Var}(b_{ij})x_j^2 \ .$$

Notice that if either p or q is odd, then

$$\int_R x_i^p x_j^q d\underline{x} = 0$$

from the symmetry of R. Therefore,

$$\Omega\int_R V_i^* d\underline{x} = \mathrm{Var}(b_i) + a[4\mathrm{Var}(b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} \mathrm{Var}(b_{ij})] \qquad (18)$$

where

$$a = \Omega\int_R x_i^2 d\underline{x} \ .$$

From equation (14) and

$$\int_R x_i^p x_j^q d\underset{\sim}{x} = 0$$

if p or q is odd, we can obtain

$$\Omega\int_R \bar{V}^* d\underset{\sim}{x} = \frac{1}{p} \sum_{i=1}^{p} [\mathrm{Var}(b_i) + a(4\mathrm{Var}(b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} \mathrm{Var}(b_{ij}))] \, . \tag{19}$$

To show

$$\int_R \bar{V}^* d\underset{\sim}{x} = \int_R V_i^* d\underset{\sim}{x}$$

for an arbitrary i , it is necessary and sufficient to have from equations (18) and (19) that

$$\mathrm{Var}(b_i) + a[4\mathrm{Var}(b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} \mathrm{Var}(b_{ij})] \tag{20}$$

are equal for all i . Theorem 1 says that if a design is slope-rotatable,

$$4\mathrm{Var}(b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} \mathrm{Var}(b_{ij})$$

are equal for all i . Additionally, if $\mathrm{Var}(b_i)$ are equal for all i , then equation (20) is true. Hence, the theorem is proved.
Q. E. D.

Suppose Q represents the class of $\hat{y}$-rotatable designs and S represents the class of slope-rotatable designs. We know that Q is a subset of S from Corollary 1. Now we consider an interesting class of designs which contains most of the useful designs known and which are fairly easy to construct. Let C denote the class of designs which satisfies the following four conditions.

1. All odd moments are zero.
2. All pure second moments are equal.
3. All pure fourth moments are equal.
4. All mixed fourth moments are equal.

Then the following relationship is true.

Corollary 4: $Q \subset C \subset S$.

Proof: The relationship $Q \subset C$ is immediate since the four conditions for C are simply part of the necessary conditions of $\hat{y}$-rotatable designs, Q . The relationship $C \subset S$ follows from Corollary 3 since the second and third conditions for C imply that $\mathrm{Var}(b_{ii})$ are equal for all i . Q. E. D.

Corollary 4 shows that the class of $\hat{y}$-rotatable designs is a subset of C and C is a subset of the class of slope-rotatable designs.

Now we want to investigate the moment matrix of C and its properties, partly because C is an important class of designs and partly because the moment matrix of S has not been found explicitly. Assume $[i^2] = a$, $[i^4] = b$ and $[i^2 j^2] = c$. The moment matrix of C is of the form:

$$
N^{-1}X'X =
\begin{array}{c}
\begin{array}{cccc} & x_1 \; x_2 \; \cdots \; x_p & x_1^2 \; x_2^2 \; \cdots \; x_p^2 & x_1x_2 \; x_1x_3 \; \cdots \; x_{p-1}x_p \end{array} \\
\left[\begin{array}{c|cccc|cccc|cccc}
1 & & * & & & a & a & \cdots & a & & * & & \\ \hline
 & a & 0 & \cdots & 0 & & & & & & & & \\
 & & a & \cdots & 0 & & * & & & & * & & \\
 & & & \ddots & \vdots & & & & & & & & \\
 & & & & a & & & & & & & & \\ \hline
 & & & & & b & c & \cdots & c & & & & \\
 & & & & & & b & \cdots & c & & * & & \\
 & & & & & & & \ddots & \vdots & & & & \\
 & & & & & & & & b & & & & \\ \hline
 & & & & & & & & & c & 0 & \cdots & 0 \\
 & & \text{(symmetric)} & & & & & & & & c & \cdots & 0 \\
 & & & & & & & & & & & \ddots & \vdots \\
 & & & & & & & & & & & & c
\end{array}\right]
\end{array}
$$

where the asterisks indicate null submatrices. The inverse matrix can be obtained from Box and Hunter (5) and the variances and covariances of the estimated coefficients for a design in C are given by

$$
\frac{N\,\mathrm{Var}(b_0)}{\sigma^2} = \frac{(b-c)[(b-c)+pc]}{A} \; ; \quad \frac{N\,\mathrm{Var}(b_i)}{\sigma^2} = \frac{1}{a} \; ;
$$

$$
\frac{N\,\mathrm{Var}(b_{ii})}{\sigma^2} = \frac{b+(p-2)c-(p-1)a^2}{A} \; ; \quad \frac{N\,\mathrm{Var}(b_{ij})}{\sigma^2} = \frac{1}{c} \; ; \qquad (21)
$$

$$
\frac{N\,\mathrm{Cov}(b_0, b_{ii})}{\sigma^2} = \frac{-a(b-c)}{A} \; ; \quad \frac{N\,\mathrm{Cov}(b_{ii}, b_{jj})}{\sigma^2} = \frac{a^2-c}{A}
$$

and all the remaining covariances are zero. Thus all first and second degree coefficients are uncorrelated except the quadratic coefficients. In equation (21) p is the number of variables and $A = (b-c)((b-c) + p(c-a^2))$.

From the fact that C is slope-rotatable the variance function for a design in C can be obtained from equation (15) and (21),

$$V(\underline{x}) = \frac{N}{\sigma^2} \bar{\bar{V}}^*$$

$$= \frac{N}{\sigma^2} [\frac{1}{p} \sum_{i=1}^{p} \mathrm{Var}(b_i) + \frac{1}{p}(4\mathrm{Var}(b_{ii}) + \sum_{\substack{j=1 \\ j\neq i}}^{p} \mathrm{var}(b_{ij})) \sum_{i=1}^{p} x_i^2]$$

$$= \frac{1}{a} + [\frac{4(b+(p-2)c-(p-1)a^2)}{pA} + \frac{p-1}{cp}] \sum_{i=1}^{p} x_i^2$$

$$= \frac{1}{a} + K\rho^2$$

where

$$\rho^2 = \sum_{i=1}^{p} x_i^2$$

and

$$K = \frac{4(b+(p-2)c-(p-1)a^2)}{pA} + \frac{p-1}{cp} .$$

$K > 0$ can be shown and this indicates that $V(\underline{x})$ is an increasing function of ρ . This result should be true since C is slope-rotatable and the variance function of any slope-rotatable design is an increasing function of ρ. If $A = (b-c)((b-c)+p(c-a^2))$ is zero, then the moment matrix is singular and some of the coefficients of the design are not estimable. $A = 0$ implies that $b = c$ or $b - c = p(a^2 - c)$, that is

$$[i^4] = [i^2j^2] \quad \text{or} \quad [i^4] - [i^2j^2] = p([i^2]^2 - [i^2j^2]) \; . \tag{22}$$

When one constructs a design which belongs to C, one should check equation (22) to avoid singularity.

3.1.2 Second Order Slope-Rotatable Designs

We have shown the precision matrix conditions which a second order design must satisfy to obtain constant slope-precision on spheres centered at the origin of the design. We now consider the problem of finding arrangements of experimental points which satisfy these conditions. The classes of slope-rotatable designs we present are by no means exhaustive but rather are intended to illustrate some of the possibilities.

From Corollary 1 any $\hat{y}$-rotatable design is slope-rotatable. Therefore, the $\hat{y}$-rotatable designs which are presented in the paper of Box and Hunter (5) are slope-rotatable. These slope-rotatable designs are not discussed here. In order to discover some of the slope-rotatable designs which are not $\hat{y}$-rotatable, we now consider arrangement of points which are equally spaced on circles, spheres or hyperspheres, *i.e.*, regular figures. Our study begins with the two dimensional figures.

Two dimensional designs: Suppose n points are equally spaced on a circle with radius ρ. The coordinates of experimental points are

$$\begin{array}{cc} x_1 & x_2 \end{array}$$

$$\begin{bmatrix} \rho\ \cos\ \alpha & \rho\ \sin\ \alpha \\ \rho\ \cos\ (\theta+\alpha) & \rho\ \sin\ (\theta+\alpha) \\ \rho\ \cos\ (2\theta+\alpha) & \rho\ \sin\ (2\theta+\alpha) \\ \vdots & \vdots \\ \rho\ \cos\ ((n-1)\theta+\alpha) & \rho\ \sin((n-1)\theta+\alpha) \end{bmatrix}$$

where α is the angle of a point on the circle measured counter-clockwise from the positive x_1 axis, and $\theta = 2\pi/n$. Any $p^{\underline{th}}$ order moment, $[1^{p-q}2^{q}]$, where p and q are non-negative integers and $p \geq q$, can be expressed as

$$M = \frac{1}{n}\,[\rho^{p} \sum_{\mu=0}^{n-1} [\cos(\mu\theta+\alpha)]^{p-q}[\sin(\mu\theta+\alpha)]^{q}] \; .$$

We may write

$$[\cos(\mu\theta+\alpha)]^{p-q} = [\frac{e^{i(\mu\theta+\alpha)} + e^{-i(\mu\theta+\alpha)}}{2}]^{p-q}$$

$$= 2^{-(p-q)} \sum_{t=0}^{p-q} \binom{p-q}{t} e^{i(\mu\theta+\alpha)(p-q-2t)}$$

and

$$[\sin(\mu\theta+\alpha)]^{q} = [\frac{e^{i(\mu\theta+\alpha)} - e^{-i(\mu\theta+\alpha)}}{2i}]^{q}$$

$$= (2i)^{-q} \sum_{r=0}^{q} \binom{q}{r} e^{i(\mu\theta+\alpha)(q-2r)}(-1)^{r} \; .$$

With the above substitutions the $p^{\underline{th}}$ order moment may be expressed as

$$M = \frac{1}{n}\left(\frac{\rho}{2}\right)^p\left(\frac{1}{i}\right)^q \sum_{\mu=0}^{n-1} \sum_{t=0}^{p-q} \sum_{r=0}^{q} (-1)^r \binom{p-q}{t}\binom{q}{r} e^{i\mu\theta(p-2t-2r)} \cdot$$

$$e^{i\alpha(p-2t-2r)} \ .$$

If the term

$$\sum_{t=0}^{p-q} \sum_{r=0}^{q} (-1)^r \binom{p-q}{t}\binom{q}{r} e^{i\mu\theta(p-2t-2r)} \cdot e^{i\alpha(p-2t-2r)}$$

were written out in a rectangular array with the terms in r running laterally and the terms in t vertically, the summation could be preformed diagonally and the result expressed as

$$\sum_{m=0}^{p} A_m e^{i\mu\theta(p-2m)} e^{i\alpha(p-2m)}$$

where $m = t + r$; $m = 0, 1, 2, \ldots, p$, and

$$A_m = \sum_{j=0}^{m} (-1)^{m-j} \binom{p-q}{j}\binom{q}{m-j} \ .$$

Therefore, with the understanding that $\binom{\alpha}{\beta} = 0$ for $\alpha < \beta$, M may be written as

$$M = K \sum_{\mu=0}^{n-1} \sum_{m=0}^{p} A_m e^{i\mu\theta(p-2m)} e^{i\alpha(p-2m)} \tag{23}$$

where $K = (\rho/2)^p (1/i)^q / n$. Examining the terms in equation (23), it is seen that $M = 0$ if $p - 2m \neq nI$, I an integer, since then

$$\sum_{\mu=0}^{n-1} e^{i\mu\theta(p-2m)} = 0$$

by the property of the summation of roots of unity. $M = 0$ also if $p - 2m = 0$, since then $A_m = 0$.

Table 3 Odd moments table

Degree	Odd Moments	n=2	n=3	n=4	n=5	n≥6
p = 1	[1],[2]	0[a]	0	0	0	0
p = 2	[12]	X[b]	0	0	0	0
p = 3	$[1^3],[2^3],[1^2 2],[12^2]$	0	X	0	0	0
p = 4	$[1^3 2],[12^3]$	X	0	X	0	0
p = 5	$[1^5],[1^4 2],[1^3 2^2],[12^4],[2^5]$	0	X	0	X	0

[a]0 = vanishes

[b]X = not vanishes

For example, let us find [12] for $n = 4$. In this case $p = 2$, $q = 1$ and $m = 0, 1$ and 2 . Notice that $p - 2m$ could be $2, 0$ and -2 as m becomes $0, 1$ and 2 , respectively. When $p - 2m = 2$ or -2 ,

$$\sum_{\mu=0}^{n-1} e^{i\mu\theta(p-2m)} = 0$$

since $p - 2m \neq 4I$, and when $p - 2m = 0$, $A_m = 0$ since

$$A_m = A_1 = \sum_{j=0}^{1} (-1)^{1-j}\binom{1}{j}\binom{1}{1-j} = -1 + 1 = 0 .$$

Consequently, $M = 0$ which indicates $[12] = 0$. In the same fashion we can construct the above odd moments table from equation (23) to show which odd moments do and do not vanish. Table 3 gives valuable information to construct the moment matrix for a design whose experimental points are equally spaced on circles.

For the first four illustrations of slope-rotatable designs we consider arrangements with n_0 points at the design center, n_1 points equally spaced on a circle of radius ρ_1 and n_2 points equally spaced on a different circle of radius ρ_2. Assume α is the angle of a point on the circle of radius ρ_1 from the positive x_1 axis and β is that of the other circle.

For the <u>first</u> illustration suppose $n_1 = 3$, $n_2 = 3$ and n_0 is arbitrary. Total observations are $N = 6 + n_0$. From Table 3 it is seen that $[1] = [2] = [12] = [1^3 2] = [12^3] = 0$. It can be shown that the moment matrix for such an arrangement is

$$N^{-1}X'X = \begin{array}{c} \begin{array}{cccccc} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & a & a & 0 \\ & a & 0 & b & -b & -c \\ & & a & -c & c & -b \\ & & & 3d & d & 0 \\ & \text{(symmetric)} & & & 3d & 0 \\ & & & & & d \end{bmatrix} \end{array}$$

where

$$a = \frac{3}{2N}(\rho_1^2 + \rho_2^2) ,$$

$$b = \frac{3}{4N}(\rho_1^3 \cos 3\alpha + \rho_2^3 \cos 3\beta) ,$$

$$c = \frac{3}{4N}(\rho_1^3 \sin 3\alpha + \rho_2^3 \sin 3\beta) ,$$

and

$$d = \frac{3}{8N}(\rho_1^4 + \rho_2^4) .$$

The inverse matrix can be shown to be

$$N(X'X)^{-1} = \begin{bmatrix} \frac{2d}{2d-a^2} & 0 & 0 & \frac{-a}{2(2d-a^2)} & \frac{-a}{2(2d-a^2)} & 0 \\ & \frac{d}{B} & 0 & \frac{-b}{2B} & \frac{b}{2B} & \frac{c}{B} \\ & & \frac{d}{B} & \frac{c}{2B} & \frac{-c}{2B} & \frac{b}{B} \\ & & & e & f & 0 \\ & \text{(symmetric)} & & & e & 0 \\ & & & & & \frac{a}{B} \end{bmatrix} \tag{24}$$

where

$$B = a(d - \frac{b^2 + c^2}{a})$$

$$e = \frac{3d - (a^2 + \frac{b^2 + c^2}{a})}{4(2d - a^2)(d - \frac{b^2 + c^2}{a})} ,$$

and

$$f = \frac{(a^2 - \frac{b^2 + c^2}{a}) - d}{4(2d - a^2)(d - \frac{b^2 + c^2}{a})} .$$

From equation (24) it is verified that this arrangement of points supply usable slope-rotatable designs as long as

$$(2d - a^2)(d - \frac{b^2 + c^2}{a}) \neq 0 \text{ .}$$

If $2d - a^2 = 0$ or $d - (b^2 + c^2)/a = 0$, then the moment matrix is singular. It can be shown that

$$(2d - a^2)(d - \frac{b^2 + c^2}{a}) \neq 0 \qquad \text{if} \qquad \rho_1 \neq \rho_2 \text{ .}$$

Therefore, the conclusion is that the above arrangement provides useful slope-rotatable designs for any number of center points and any angles of α and β if $\rho_1 \neq \rho_2$. Note that such an arrangement of points does not supply a $\hat{y}$-rotatable design or a design in C , simply because b and c cannot be zero at the same time.

For the second illustration consider $n_1 = 4$, $n_2 = 4$ and n_0 is arbitrary. We have $N = 8 + n_0$. From Table 3 [1] , [2] , [12] , $[1^3]$, $[2^3]$, $[1^2 2]$, and $[12^2]$ are all zero. The moment matrix of this arrangement is readily shown to be

$$N^{-1}X'X = \begin{array}{c} \begin{array}{cccccc} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 2a & 2a & 0 \\ & 2a & 0 & 0 & 0 & 0 \\ & & 2a & 0 & 0 & 0 \\ & & & b & c & d/2 \\ & & & & b & -d/2 \\ & \text{(symmetric)} & & & & c \end{bmatrix} \end{array} \qquad (25)$$

where

$$a = \frac{\rho_1^2 + \rho_2^2}{N} \text{ ,}$$

$$b = \frac{\rho_1^4(1 + \cos^2 2\alpha) + \rho_2^4(1 + \cos^2 2\beta)}{N},$$

$$c = \frac{\rho_1^4 \sin^2 2\alpha + \rho_2^4 \sin^2 2\beta}{N};$$

and

$$d = \frac{\rho_1^4 \sin 4\alpha + \rho_2^4 \sin 4\beta}{N}.$$

The inverse matrix is given by

$$N(X'X)^{-1} = \begin{bmatrix} \frac{b+c}{b+c-8a^2} & 0 & 0 & \frac{-2a}{b+c-8a^2} & \frac{-2a}{b+c-8a^2} & 0 \\ & \frac{1}{2a} & 0 & 0 & 0 & 0 \\ & & \frac{1}{2a} & 0 & 0 & 0 \\ & & & e & f & \frac{-d}{2(c(b-c)-\frac{1}{2}d^2)} \\ & \text{(symmetric)} & & & e & \frac{+d}{2(c(b-c)-\frac{1}{2}d^2)} \\ & & & & & \frac{b-c}{c(b-c)-\frac{1}{2}d^2} \end{bmatrix}$$

where

$$e = \frac{c(b-a^2) - d^2/4}{T},$$

$$f = \frac{c(4a^2 - c) - d^2/4}{T},$$

and

$$T = (b + c - 8a^2)(c(b - c) - d^2/2) ,$$

which implies that the slope-rotatable conditions are satisfied. An important point to note here is that if the quantity T is zero, then certain of the variances and covariances are infinite. This can be attributed to $|X'X|$ being zero, thus yielding a useless design. This will occur when $b + c - 8a^2 = 0$ or $c(b - c) - d^2/2 = 0$. The quantity $b + c - 8a^2$ is zero if $\rho_1 = \rho_2$ and $n_0 = 0$, and the quantity $c(b - c) - d^2/2$ is zero if $\alpha - \beta = \frac{\pi}{2} \cdot I$, I an integer. Therefore, we conclude that the above arrangement supplies usable slope-rotatable designs unless $\alpha - \beta = \frac{\pi}{2} \cdot I$, I is an integer, or $\rho_1 = \rho_2$ in case of $n_0 = 0$.

In the moment matrix equation (25) d is zero if $\rho_1^4 \sin 4\alpha + \rho_2^4 \sin 4\beta = 0$. For instance, if $\alpha = 0^\circ$ and $\beta = 45^\circ$, then $d = 0$ for any ρ_1 and ρ_2. If $d = 0$, then the moment matrix is nothing but that of C. In addition to $d = 0$, if $b = 3c$, a $\hat{y}$-rotatable configuration is obtained. In fact, if $\rho_1 = \rho_2$, $\alpha - \beta = \frac{\pi}{4}$ and $n_0 > 0$, then this arrangement supplies a useful class of $\hat{y}$-rotatable designs, namely rotatable central composite designs.

For the <u>third</u> illustration of the equiradial arrangement consider $n_1 \geq 5$ and $n_2 = 3$. We have $N = 3 + n_1 + n_0$. Noticing that all odd moments up to $p = 4$ are zero in case of $n \geq 5$, we obtain the following moment matrix for this arrangement.

$$
N^{-1}X'X = \begin{array}{c} \\ \\ \end{array}
\begin{array}{cccccc}
 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \\
\end{array}
$$

$$
N^{-1}X'X = \begin{bmatrix}
1 & 0 & 0 & a & a & 0 \\
 & a & 0 & b & -b & -c \\
 & & a & -c & c & -b \\
 & & & 3d & d & 0 \\
 & \text{(symmetric)} & & & 3d & 0 \\
 & & & & & d
\end{bmatrix}
$$

where

$$a = \frac{n_1\rho_1^2 + 3\rho_2^2}{2N} ,$$

$$b = \frac{3\rho_1^3 \cos 3\beta}{4N} ,$$

$$c = \frac{3\rho_1^3 \sin 3\beta}{4N} ,$$

and

$$d = \frac{n_1\rho_1^4 + 3\rho_2^4}{8N} .$$

The inverse matrix has the same form as that of the first illustration, equation (24). Therefore, this arrangement provides usable slope-rotatable designs.

As the fourth illustration of the equiradial arrangement, consider $n_1 \geq 5$, $n_2 = 4$ and n_0 is arbitrary. Similarly, it can be show that this arrangement provides usable slope-rotatable designs.

Up to now we have presented four classes of designs which consist of two circles and center points. As the last example for two independent variables, we will consider the following configuration given by the design matrix with $N = 8 + n_0$, where n_0 is the number of center points.

$$
\begin{array}{ccc}
 & \begin{array}{cc} x_1 & x_2 \end{array} & \\
D_m = & \left[\begin{array}{cc}
a_1 & a_2 \\
a_1 & -a_2 \\
-a_1 & a_2 \\
-a_1 & -a_2 \\
a_3 & 0 \\
-a_3 & 0 \\
0 & a_4 \\
0 & -a_4 \\
0 & 0 \\
0 & 0 \\
\vdots & \vdots \\
0 & 0
\end{array}\right] &
\begin{array}{l}
\\ \\ \\ \cdots \ 8 \text{ trials} \\ \\ \\ \\ \\ \\ \cdots \ n_0 \text{ trials} \\ \\ \\
\end{array}
\end{array}
$$

The moment matrix for this arrangement is

$$N^{-1}X'X = \begin{array}{cccccc} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \\ \end{array}$$

$$N^{-1}X'X = \begin{bmatrix} 1 & 0 & 0 & \frac{4a_1^2+2a_3^2}{N} & \frac{4a_2^2+2a_4^2}{N} & 0 \\ & \frac{4a_1^2+2a_3^2}{N} & 0 & 0 & 0 & 0 \\ & & \frac{4a_2^2+2a_4^2}{N} & 0 & 0 & 0 \\ & & & \frac{4a_1^4+2a_3^4}{N} & \frac{4a_1^2a_2^2}{N} & 0 \\ & \text{(symmetric)} & & & \frac{4a_2^4+2a_4^4}{N} & 0 \\ & & & & & \frac{4a_1^2a_2^2}{N} \end{bmatrix} \tag{27}$$

The inverse matrix is simple to find from equation (27), hence it is not written here. From Corollary 3, $\mathrm{Var}(b_{11})$ should be equal to $\mathrm{Var}(b_{22})$ for slope-rotatability. Let

$$\mathrm{Det} = \begin{vmatrix} 1 & \frac{4a_1^2+2a_3^2}{N} & \frac{4a_2^2+2a_4^2}{N} \\ & \frac{4a_1^4+2a_3^4}{N} & \frac{4a_1^2a_2^2}{N} \\ \text{(symmetric)} & & \frac{4a_2^4+2a_4^4}{N} \end{vmatrix} .$$

From the moment matrix equation (27), $\mathrm{Var}(b_{11}) = \mathrm{Var}(b_{22})$ if and only if

$$\left(\frac{4a_1^4+2a_3^4}{N}\right) - \left(\frac{4a_1^2+2a_3^2}{N}\right)^2 = \left(\frac{4a_2^4+2a_4^4}{N}\right) - \left(\frac{4a_2^2+2a_4^2}{N}\right)^2 \quad \text{and} \quad \mathrm{Det} \neq 0$$

which is simplified to

$$N[2(a_1^4-a_2^4) + (a_3^4-a_4^4)] = 2[2(a_1^2+a_2^2) + (a_3^2+a_4^2)] \cdot$$

$$[2(a_1^2-a_2^2) + (a_3^2-a_4^2)] \tag{28}$$

and $\text{Det} \neq 0$. In other words, equation (28) is the necessary and sufficient condition for slope-rotatability for this arrangement. For equation (28) to be true for an arbitrary N , the following conditions should hold.

1. $2(a_1^4-a_2^4) + (a_3^4-a_4^4) = 0$,

2. $2(a_1^2-a_2^2) + (a_3^2-a_4^2) = 0$, (29)

3. $\text{Det} \neq 0$.

Notice that, for a design in this arrangement to belong to the class of designs C , equations (29) is also necessary and sufficient, which can be seen from the moment matrix equation (27) since the first condition in equation (29) is obtained from $[1^2] = [2^2]$ and the next one from $[1^4] = [2^4]$. For example, with $n_0 \geq 0$, $(a_1, a_2, a_3, a_4) = (\sqrt{2}, 2, \sqrt{5}, 1)$ or $(\sqrt{2}, 1, \sqrt{1/2}, \sqrt{5/2})$ gives a usable design belonging to C . Obviously there are infinite number of possible designs belonging to C in this arrangement. Recall that any design in C is slope-rotatable.

What are the conditions needed for this arrangement to give $\dot{y}$-rotatability? From Box and Hunter it is known that $[1^2] = [2^2]$ and

$[1^4] = [2^4] = 3[1^2 2^2]$ are required to achieve $\hat{y}$-rotatability. Therefore, we can obtain from equation (27) that

$$2(a_1^2 - a_2^2) + (a_3^2 - a_4^2) = 0 \qquad \text{from} \qquad [1^2] = [2^2] \ ,$$

$$2(a_1^4 - a_2^4) + (a_3^4 - a_4^4) = 0 \qquad \text{from} \qquad [1^4] = [2^4] \ , \tag{30}$$

and

$$2a_1^4 + a_3^4 = 6a_1^2 a_2^2 \qquad \text{from} \qquad [1^4] = 3[1^2 2^2] \ .$$

Also we need $\text{Det} \neq 0$ for non-singularity of $X'X$. For instance, $a_1 = a_2$, $a_3 = a_4 = \sqrt{2}\, a_1$ and $n_0 > 0$ supplies a $\hat{y}$-rotatable design. Notice that equation (30) satisfies equation (29), which should be true since the class of $\hat{y}$-rotatable designs is a subset of $\mathcal{G}$.

Three dimensional designs: Box and Hunter (5) developed a number of $\hat{y}$-rotatable second order designs in three dimensions. Among them three basic $\hat{y}$-rotatable designs are: one based on the icosahedron, a 12 pointed, 20 sided regular figure with additional points at the center; a second based on the dodecahedron which has 20 points and 12 faces; and a third design based on a cube and an octahedron concentrically placed. Box and Hunter showed for each case that some strict relationships should hold among the coordinates of experimental points in order to give $\hat{y}$-rotatability. We now want to show that for the three designs above the conditions needed for $\hat{y}$-rotatability are not necessary for slope-rotatability. In other words, we will illustrate three design configurations which are slope-rotatable but may not be $\hat{y}$-rotatable.

The first illustration is the design configuration based on the icosahedron, whose design matrix is

$$D_m = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} 0 & a_1 & a_2 \\ 0 & a_1 & -a_2 \\ 0 & -a_1 & a_2 \\ 0 & -a_1 & -a_2 \\ a_2 & 0 & a_1 \\ -a_2 & 0 & a_1 \\ -a_2 & 0 & -a_1 \\ a_2 & 0 & -a_1 \\ a_1 & a_2 & 0 \\ a_1 & -a_2 & 0 \\ -a_1 & a_2 & 0 \\ -a_1 & -a_2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \end{bmatrix} \end{array}$$

where there are n_0 center points. The moments of this configuration are given by

$$[i^2] = 4(a_1^2 + a_2^2)/N \quad \text{for all} \quad i \; ,$$

$$[i^4] = 4(a_1^4 + a_2^4)/N \quad \text{for all} \quad i \; ,$$

$$[i^2 j^2] = 4a_1^2 a_2^2/N \quad \text{for any } i \text{ and } j \text{ where } i \neq j \ ,$$

and all odd moments $= 0$.

The matrix of these moments is exactly the same form as that of C , so that this design configuration supplies slope-rotatable designs for any a_1 and a_2 . To be $\hat{y}$-rotatable the ratio, a_1/a_2 , should be 1.618 . This ratio condition is not necessary for slope-rotatability.

The second illustration is the design configuration based on the dodecahedron, whose design matrix, with n_0 center points, is given below. The moments of this configurations are

$$[i^2] = (8 + 4c^2 + 4/c^2)/N \quad \text{for all } i \ ,$$

$$[i^4] = (8 + 4c^4 + 4/c^4)/N \quad \text{for all } i \ ,$$

$$[i^2 j^2] = 12/N \quad \text{for any } i \text{ and } j \text{ where } i \neq j \ ,$$

and all odd moments $= 0$.

The matrix of these moments is also of the form of C , hence the configuration gives slope-rotatable designs. To be $\hat{y}$-rotatable, c must be 1.618 which is not a necessary condition for slope-rotatability.

$$
D_m = \begin{array}{c} \begin{matrix} x_1 & x_2 & x_3 \end{matrix} \\ \begin{bmatrix}
0 & 1/c & c \\
0 & -1/c & c \\
0 & 1/c & -c \\
0 & -1/c & -c \\
c & 0 & 1/c \\
-c & 0 & -1/c \\
-c & 0 & 1/c \\
c & 0 & -1/c \\
1/c & c & 0 \\
-1/c & -c & 0 \\
-1/c & c & 0 \\
1/c & -c & 0 \\
-1 & -1 & -1 \\
1 & -1 & -1 \\
-1 & 1 & -1 \\
-1 & -1 & 1 \\
1 & -1 & 1 \\
1 & 1 & -1 \\
-1 & 1 & 1 \\
1 & 1 & 1 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\vdots & \vdots & \vdots \\
0 & 0 & 0
\end{bmatrix} \end{array}
$$

The third illustration is based on a cube and an octahedron concentrically placed. The design matrix is given by

$$
D_m = \begin{array}{c}
\begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\
\left[\begin{array}{ccc}
-a & -a & -a \\
a & -a & -a \\
-a & a & -a \\
a & a & a \\
-a & -a & a \\
a & -a & a \\
-a & a & a \\
a & a & a \\
-b & 0 & 0 \\
b & 0 & 0 \\
0 & -b & 0 \\
0 & b & 0 \\
0 & 0 & -b \\
0 & 0 & b \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\vdots & \vdots & \vdots \\
0 & 0 & 0
\end{array}\right]
\end{array}
\begin{array}{l}
\\ \\ \\ \\ \cdots \text{ Cube} \\ \\ \\ \\ \\ \\ \\ \cdots \text{ Octahedron} \\ \\ \\ \\ \\ \\ \cdots \text{ Center} \\ \\
\end{array}
$$

The moment matrix is easy to obtain and it indicates that the design configuration also gives slope-rotatable designs. To be $\hat{y}$-rotatable, the ratio, b/a , should be $2^{3/4} \doteq 1.682$, which is not necessary for slope-rotatability. Any ratio of b/a produces a slope-rotatable design.

<u>More than three dimensional designs</u>: There are few regular figures in more than three dimensions which may be practically useful in the formation of slope-rotatable designs. They are the hypercube of 2^p points (p-dimensional analogue of the cube), the cross polytope of $2p$ points (p-dimensional analogue of the octahedron) and a $2^p + 2p$ pointed figure (*i.e.*, central composite designs) which is a combination of the two. Central composite designs have the design matrix

$$D_m = \begin{array}{c} \\ \\ \end{array}\begin{array}{cccccc} x_1 & x_2 & \cdot & \cdot & \cdot & x_p \end{array}$$

$$D_m = \left[\begin{array}{cccccc} a & a & \cdot & \cdot & \cdot & a \\ a & a & \cdot & \cdot & \cdot & -a \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -a & -a & \cdot & \cdot & \cdot & -a \\ b & 0 & \cdot & \cdot & \cdot & \cdot \\ -b & 0 & \cdot & \cdot & \cdot & \cdot \\ 0 & b & \cdot & \cdot & \cdot & \cdot \\ 0 & -b & \cdot & \cdot & \cdot & \cdot \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdot & \cdot & \cdot & b \\ 0 & 0 & \cdot & \cdot & \cdot & -b \\ 0 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & \cdot & \cdot & \cdot & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdot & \cdot & \cdot & 0 \end{array}\right] \begin{array}{l} \\ \\ \cdot\ \cdot\ \text{Hypercube} \\ \\ \\ \\ \\ \\ \\ \cdot\ \cdot\ \text{Cross Polytope} \\ \\ \\ \\ \\ \cdot\ \cdot\ \text{Center} \\ \\ \end{array}$$

where $N = 2^p + 2p + n_0$. The moment matrix of this arrangement indicates that it supplies slope-rotatable designs for any ratio of b/a . Note that b/a should be $2^{p/4}$ to be $\hat{y}$-rotatable.

3.2 Designs for the Quadratic Model When the True Model is Cubic

In the previous section the emphasis has been on the use of slope-rotatable designs for fitting second order models assuming the fitted models describe the true response functions properly. In many cases the fitted polynomial is not exactly adequate. Therefore, equally important is the consideration of the bias due to the inadequacy of the model.

In this section we discuss quadratic polynomial designs, in several variables, which afford protection against the existence of cubic terms in the true response function. The equation of the fitted model is $\hat{y}(\underline{x}) = \underline{x}_1'\underline{b}_1$ in which $\underline{x}_1$ and $\underline{b}_1$ take the forms in Section 3.1 and the true relationship is $\eta(\underline{x}) = \underline{x}_1'\underline{\beta}_1 + \underline{x}_2'\underline{\beta}_2$ where $\underline{x}_2' = (x_1^3, x_2^3, \ldots, x_p^3; x_1^2x_2, x_1^2x_3, \ldots, x_p^2x_{p-1})$ and the vector $\underline{\beta}_2$ contains the coefficients corresponding to terms in $\underline{x}_2'$; terms such as $\beta_{111}, \beta_{222}, \ldots$ are included.

The effect of bias on designing experiments and its properties can be explained well by examining two illustrative examples in detail. Two particular classes of designs for two independent variables are studied; one class is the designs whose points are equally spaced on a circle with center points, and the other class is the designs with two circles with four points on each circle plus center points. Notice that for two independent variables X_2 and D_2 take the forms;

$$X_2 = \begin{bmatrix} x_{11}^3 & x_{21}^3 & x_{11}^2 x_{21} & x_{11} x_{21}^2 \\ x_{12}^3 & x_{22}^3 & x_{12}^2 x_{22} & x_{12} x_{22}^2 \\ \vdots & \vdots & \vdots & \vdots \\ x_{1N}^3 & x_{2N}^3 & x_{1N}^2 x_{2N} & x_{1N} x_{2N}^2 \end{bmatrix}$$

and

$$D_2 = \begin{bmatrix} 3x_1^2 & 0 & 2x_1 x_2 & x_2^2 \\ 0 & 3x_2^2 & x_1^2 & 2x_1 x_2 \end{bmatrix} .$$

The matrices X_1 and D_1 are given previously in Section 3.1.

The reasons why we choose the two illustrations above are as follows. First, they are commonly known designs. In particular, the first class contains the hexagonal design and the $\hat{y}$-rotatable central composite design, and the latter class contains the 3^2 symmetric factorial design, all of which are very useful in response surface experimentation. Secondly, they are slope-rotatable designs. Finally, they supply optimal or near-optimal designs under some conditions, which will be discussed in the next chapter.

3.2.1 Designs With Points Equally Spaced on a Single Circle

For the case of two independent variables, the equation of the fitted model is

$$\hat{y}(\underline{x}) = b_0 + b_1x_1 + b_2x_2 + b_{11}x_1^2 + b_{22}x_2^2 + b_{12}x_1x_2$$

and the true response function is

$$\eta(\underline{x}) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \beta_{12}x_1x_2$$

$$+ \beta_{111}x_1^3 + \beta_{222}x_2^3 + \beta_{112}x_1^2x_2 + \beta_{122}x_1x_2^2 ,$$

hence,

$$\underline{x}_2' = (x_1^3, x_2^3, x_1^2x_2, x_1x_2^2)$$

and

$$\underline{\beta}_2' = (\beta_{111}, \beta_{222}, \beta_{112}, \beta_{122}) .$$

Suppose the experimenter wants to place $n_1 \geq 6$ equally spaced points on a circle of radius ρ, augmented by $n_0 \geq 1$ center points. If α_1 is the rotation of a design point on the circle from the positive x_1-axis, then the design matrix can be written as

$$\begin{array}{cc}
x_1 & x_2 \\
\rho \cos \alpha_1 & \rho \sin \alpha_1 \\
\rho \cos (\theta+\alpha_1) & \rho \sin (\theta+\alpha_1) \\
\rho \cos (2\theta+\alpha_1) & \rho \sin (2\theta+\alpha_1) \\
\vdots & \vdots \\
\rho \text{ dos } ((n_1-1). & \rho \sin ((n_1-1). \\
\theta+\alpha_1) & \theta+\alpha_1)
\end{array}$$

where $\theta = 2\pi/n_1$. It is of interest now to investigate the moment matrix and the precision matrix for such designs. These matrices are obtained as below.

$$
N^{-1}X_1'X_1 = \begin{array}{c}
\begin{matrix} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{matrix} \\
\begin{bmatrix}
1 & 0 & 0 & \rho^2 f/2 & \rho^2 f/2 & 0 \\
 & \rho^2 f/2 & 0 & 0 & 0 & 0 \\
 & & \rho^2 f/2 & 0 & 0 & 0 \\
 & & & 3\rho^4 f/8 & \rho^4 f/8 & 0 \\
 & \text{(symmetric)} & & & 3\rho^4 f/8 & 0 \\
 & & & & & \rho^4 f/8
\end{bmatrix}
\end{array}
$$

and

$$
N(X_1'X_1)^{-1} = \begin{array}{c}
\begin{matrix} \phantom{\frac{1}{1-f}} & b_1 & b_2 & b_{11} & b_{22} & b_{12} \end{matrix} \\
\begin{bmatrix}
\frac{1}{1-f} & 0 & 0 & \frac{-1}{(1-f)\rho^2} & \frac{-1}{(1-f)\rho^2} & 0 \\
 & \frac{2}{\rho^2 f} & 0 & 0 & 0 & 0 \\
 & & \frac{2}{\rho^2 f} & 0 & 0 & 0 \\
 & & & \frac{3-2f}{f(1-f)\rho^4} & \frac{2f-1}{f(1-f)\rho^4} & 0 \\
 & & & & \frac{3-2f}{f(1-f)\rho^4} & 0 \\
 \text{(symmetric)} & & & & & \frac{8}{\rho^4 f}
\end{bmatrix}
\end{array}
$$

where $N = n_1 + n_0$ and $f = n_1/N$, the proportion of trials on the circle to the total number of trials. It is obvious from the moment matrix that these designs are $\hat{y}$-rotatable, which implies that they are slope-rotatable.

As mentioned earlier, two types of region of interest are generally used; one is the unit square and another one is the unit circle. We discuss both cases to evaluate the design criterion J , the mean squared error integrated over R .

<u>The unit square region of interest</u>: The variance of the estimated slope at $\underline{x} = (x_1, x_2)$ along the x_1 factor axis is

$$V_1^* = \mathrm{Var}\left(\frac{\partial \hat{y}}{\partial x_1}\right)$$

$$= \mathrm{Var}(b_1 + 2b_{11}x_1 + b_{12}x_2)$$

$$= \frac{\sigma^2}{N}\left[\frac{2}{\rho^2 f} + 4x_1^2\left(\frac{3-2f}{f(1-f)\rho^4}\right) + x_2^2\left(\frac{8}{\rho^4 f}\right)\right] .$$

Since the equiradial designs are slope-rotatable and $\mathrm{Var}(b_1) = \mathrm{Var}(b_2)$, Theorem 2 can be used to evaluate V . That is,

$$V = \frac{N\Omega}{\sigma^2}\int_R V_1^* d\underline{x} \qquad \text{where} \qquad \Omega^{-1} = \int_R d\underline{x} = \int_{-1}^{1}\int_{-1}^{1} dx_1 dx_2 = 4 ,$$

$$= \frac{N}{4\sigma^2}\int_{-1}^{1}\int_{-1}^{1}\left[\frac{\sigma^2}{N}\left(\frac{2}{\rho^2 f} + 4x_1^2\left(\frac{3-2f}{f(1-f)\rho^4}\right) + x_2^2\left(\frac{8}{\rho^4 f}\right)\right]dx_1 dx_2$$

$$= \frac{2}{f\rho^2} + \frac{4(5-4f)}{3f(1-f)\rho^4} . \tag{31}$$

In order to evaluate the integrated squared bias B , the alias matrix should be found. It is readily shown to be

$$A = (X_1'X_1)^{-1}X_1'X_2 = \begin{array}{c} \begin{array}{cccc} \beta_{111} & \beta_{222} & \beta_{112} & \beta_{122} \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 0 \\ \frac{3}{4}\rho^2 & 0 & 0 & \frac{1}{4}\rho^2 \\ 0 & \frac{3}{4}\rho^2 & \frac{1}{4}\rho^2 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array} .$$

The integrated squared bias is then

$$B = \frac{N\Omega}{\sigma^2}\int_R \bar{B}^* d\underline{x}$$

$$= \frac{N\Omega}{\sigma^2}\int_R \frac{1}{2}\,\underline{s}'\underline{s}\,d\underline{x} \qquad \text{since } \bar{B}^* = \underline{s}'\underline{s}/2 \text{ from (8) ,}$$

$$= \frac{N}{4\sigma^2}\int_{-1}^{1}\int_{-1}^{1} \frac{1}{2}[(D_1A-D_2)\underline{\beta}_2]'[(D_1A-D_2)\underline{\beta}_2]dx_1dx_2 \quad \text{from (12) ,}$$

$$= \frac{N}{8\sigma^2}\int_{-1}^{1}\int_{-1}^{1}[\frac{3}{4}\rho^2\beta_{111} + \frac{1}{4}\rho^2\beta_{122} - (3x_1^2\beta_{111} + x_2^2\beta_{122}$$

$$+ 2x_1x_2\beta_{112})]^2dx_1dx_2$$

$$+ \frac{N}{8\sigma^2}\int_{-1}^{1}\int_{-1}^{1}[\frac{3}{4}\rho^2\beta_{222} + \frac{1}{4}\rho^2\beta_{112} - (3x_2^2\beta_{222} + 2x_1x_2\beta_{122}$$

$$+ x_1^2\beta_{112})]^2dx_1dx_2 . \qquad (32)$$

If we assume $\beta_{111} = \beta_{222} = \beta_{112} = \beta_{122}$, then

$$B = \frac{N\beta_{111}^2}{4\sigma^2} \int_{-1}^{1}\int_{-1}^{1} (\rho^2 - (3x_1^2 + 2x_1x_2 + x_2^2))^2 dx_1 dx_2$$

$$= \alpha^2(\rho^4 - \frac{8}{3}\rho^2 + \frac{28}{9}) \tag{33}$$

where $\alpha = \sqrt{N}\,\beta_{111}/\sigma$. Therefore, the mean squared error integrated over R is

$$J = V + B = [\frac{2}{f\rho^2} + \frac{4(5-4f)}{3f(1-f)\rho^4}] + \alpha^2(\rho^4 - \frac{8}{3}\rho^2 + \frac{28}{9}) \; . \tag{34}$$

From equation (34) it is observed that V is a monotonically decreasing function of ρ with

$$\lim_{\rho \to +\infty} V = 0 \; ,$$

and B is a convex function of ρ whose minimum is achieved at $\rho = \sqrt{4/3}$, that is, approximately 1.155 . From the behavior of V and B it is easy to see that minimum J is achieved for $1.155 \leq \rho < +\infty$ for any given α . Once ρ is fixed the minimizing value of f , f* , can be obtained by solving

$$dJ/df = 0 \; ,$$

which gives

$$f^* = \frac{3\rho^2 + 10 - \sqrt{6\rho^2 + 20}}{3\rho^2 + 8} \; .$$

Obviously the ρ which minimizes J (call this ρ^*) depends on α , and therefore, so does f^* . Table 4 shows how ρ^* and f^* vary as α changes.

Table 4 ρ^* and f^* vs. α for the unit square R

α	ρ^*	f^*	V	B	J (Optimum)
0	$\to +\infty$		$\to 0$	0	$\to 0$
1	1.577	0.7471	3.371	2.664	6.035
2	1.387	0.7374	5.224	6.728	11.952
3	1.304	0.7332	6.477	13.213	19.690
4	1.260	0.7310	7.308	22.368	29.676
$+\infty$	1.155	0.7257	9.968	$+\infty$	$+\infty$

Notice that as α gets large, ρ^* decreases approaching 1.155 and f^* also decreases approaching 0.7257 . This is the same aspect we have observed in Section 2.3. Also f^* changes very little as α changes over the entire interval. However, ρ^* changes widely. In practice, since n_1 is an integer, the optimum f^* can only be approximately achieved.

If the region of operability is limited to R , the unit square, then the largest possible ρ depends on n_1 because of the special shape of R . For instance, if $n_1 = 6$, the largest ρ is 1.035 , and if $n_1 = 7$, it is 1.006 , etc. It was found by the computer that if $n_1 \geq 6$, the largest possible ρ is less than 1.155 . Therefore, both V and B are minimized at the largest possible ρ when the region of operability is limited to R .

<u>The unit circular region of interest</u>: Using the same procedure we have used for the unit square region of interest, we can obtain the following:

Table 5 ρ^* and f^* vs. α for the unit circle R

α	ρ^*	f^*	V	B	J (Optimum)
0	$\to +\infty$		$\to 0$	0	$\to 0$
1	1.493	0.7523	3.342	2.177	5.519
2	1.297	0.7431	5.353	4.528	9.881
3	1.208	0.7378	6.831	7.898	14.729
4	1.153	0.7346	8.031	12.403	20.434
$+\infty$	1.000	0.7257	13.291	$+\infty$	$+\infty$

$$V = \frac{2}{f\rho^2} + \frac{5-4f}{f(1-f)\rho^4}$$

and

$$B = \alpha^2(\rho^4 - 2\rho^2 + \frac{5}{3}) \ , \quad \text{where} \quad \alpha = \frac{\sqrt{N}\,\beta_{111}}{\sigma} \ .$$

Consequently, $$J = V + B = [\frac{2}{f\rho^2} + \frac{5-4f}{f(1-f)\rho^4}] + \alpha^2(\rho^4 - 2\rho^2 + \frac{5}{3}) \ . \quad (35)$$

Notice the difference from the previous case that B is minimized at $\rho = 1$ and minimum J is achieved for $1 \le \rho < +\infty$. Also the minimizing f for a given ρ is,

$$f^* = \frac{2\rho^2 + 5 - \sqrt{2\rho^2 + 5}}{2\rho^2 + 4} \ .$$

Table 5 shows the variation of f^* and ρ^* as α changes. As expected, Table 5 shows similar aspects for ρ^* and f^* as we have observed in Table 4. If the points are restricted to the region R, then B is minimized at the largest possible ρ (i.e., $\rho^* = 1$) which also minimizes V term. Note that at $\rho^* = 1$, $f^* = 0.7257$.

When we calculate the integrated squared bias for the two types of region of interest, we assumed that $\beta_{111} = \beta_{222} = \beta_{112} = \beta_{122}$. What happens if the assumption is relaxed? This is an interesting problem to study, and we propose the following assertion.

<u>Theorem 3</u>: For any values of β_{111} , β_{222} , β_{112} and β_{122} for the designs with points equally spaced on a single circle in two independent variables, the integrated squared bias achieves minimum at $\rho = 1$ if the region of interest is the unit circle, and at $\rho = 1.155$ if the region of interest is the unit square.

<u>Proof</u>: The integrated squared bias is given in equation (32) as

$$B = \frac{N\Omega}{2\sigma^2} \int_R [(\tfrac{3}{4} h^2\beta_{111} + \tfrac{1}{4} h^2\beta_{122})$$

$$- (3x_1^2\beta_{111} + x_2^2\beta_{122} + 2x_1x_2\beta_{112})]^2 d\underline{x}$$

$$+ \frac{N\Omega}{2\sigma^2} \int_R [(\tfrac{3}{4} h^2\beta_{222} + \tfrac{1}{4} h^2\beta_{112})$$

$$- (3x_2^2\beta_{222} + 2x_1x_2\beta_{122} + x_1^2\beta_{112})]^2 d\underline{x}$$

$$= B_1 + B_2$$

where B_1 is the first term and B_2 is the second term in the expression of B . Suppose the region of interest is the unit circle. If $\beta_{111} \neq 0$, then B_1 can be written

$$B_1 = \frac{\alpha^2}{\pi} \int_R [(\tfrac{3}{4} \rho^2 + \tfrac{1}{4} r_1\rho^2) - (3x_1^2 + x_2^2 r_1 + 2x_1x_2r_2)]^2 dx_1dx_2$$

where $r_1 = \beta_{122}/\beta_{111}$, $r_2 = \beta_{112}/\beta_{111}$, and $\alpha = \sqrt{N}\,\beta_{111}/\sigma$. From the property that $\int_R x_1^p x_2^q dx_1 dx_2 = 0$ if p or q is odd, B_1 may be written as

$$B_1 = (\frac{3}{4} + \frac{1}{4} r_1)^2 \alpha^2 [\rho^4 - 2\rho^2 + \text{constant}]$$

which indicates that B_1 is minimized at $\rho = 1$. If $\beta_{111} = 0$, and $\beta_{122} \neq 0$, then B_1 is

$$B_1 = \frac{\alpha^2}{\pi} \int_R [\frac{1}{4} \rho^2 - (x_2^2 + 2x_1 x_2 r_3)]^2 dx_1 dx_2$$

where $r_3 = \beta_{112}/\beta_{122}$ and $\alpha = \sqrt{N}\,\beta_{122}/\sigma$. It can be shown that

$$B_1 = \frac{\alpha^2}{16} (\rho^4 - 2\rho^2 + \text{constant})$$

which also implies that B_1 is minimized at $\rho = 1$. If $\beta_{111} = \beta_{122} = 0$, then B_1 is independent of ρ , hence it is not necessary to consider this case. Similarly, we can show that B_2 is minimized at $\rho = 1$. Therefore, B is minimized at $\rho = 1$ if the region of interest is the unit circle.

Suppose the region of interest is the unit square. If $\beta_{111} \neq 0$, then

$$B_1 = \frac{\alpha^2}{4} \int_R [\frac{3}{4} \rho^2 + \frac{1}{4} r_1 \rho^2 - (3x_1^2 + x_2^2 r_1 + 2x_1 x_2 r_2)]^2 dx_1 dx_2$$

where $r_1 = \beta_{122}/\beta_{111}$, $r_2 = \beta_{112}/\beta_{111}$ and $\alpha = \sqrt{N}\,\beta_{111}/\sigma$. B_1 is then

$$B_1 = \alpha^2 (\frac{3}{4} + \frac{1}{4} r_1)^2 (\rho^4 - \frac{8}{3} \rho^2 + \text{constant})$$

which shows that B_1 is minimized at $\rho = 1.155$. If $\beta_{111} = 0$ and $\beta_{122} \neq 0$, then B_1 can be shown that

$$B_1 = \frac{\alpha^2}{16} (\rho^4 - \frac{8}{3} \rho^2 + \text{Constant}) \quad \text{where} \quad \alpha = \frac{\sqrt{N}\, \beta_{122}}{\sigma} ,$$

which is also minimized at $\rho = 1.155$. Similarly, B_2 is minimized at $\rho = 1.155$. Therefore, B is minimized at $\rho = 1.155$ if the region of interest is the unit square. Q. E. D.

Theorem 3 gives valuable information to the experimenter. If he feels that a significantly large bias exists in the quadratic model and he wants to use the single circle equiradial designs, then he might want to take ρ near 1 for the unit circular region of interest, R , and ρ near 1.155 for the unit square R , since Theorem 3 tells the experimenter that no matter what values β_{ijk}'s are, B is minimized at $\rho = 1$ for the unit circle R and at $\rho = 1.155$ for the unit square R .

3.2.2 Designs With Points Equally Spaced on Two Concentric Circles

Next consider a design with four equally spaced points on a circle of radius ρ_1 and another four equally spaced points on a different circle of radius ρ_2 , augmented by n_0 center points. If a point on the first circle makes an angle α and a point on the second circle makes an angle β with the positive x_1-axis, then the moment matrix and its inverse matrix were found in equations (25) and (26). We showed also that this class of designs is slope-rotatable. Now we want to find V , B and J explicitly to discuss their properties.

<u>The unit square region of interest</u>: If the region of interest, R, is the unit square, W_{11} is given by

$$W_{11} = \Omega \int_R D_1' D_1 d\underline{x} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ & 1 & 0 & 0 & 0 & 0 \\ & & 1 & 0 & 0 & 0 \\ & & & \frac{4}{3} & 0 & 0 \\ & & & & \frac{4}{3} & 0 \\ & \text{(symmetric)} & & & & \frac{2}{3} \end{bmatrix} .$$

By substituting W_{11} and $N(X_1'X_1)^{-1}$ of equation (26) into equation (11), it can be shown that the integrated variance is

$$V = \frac{1}{2a} + \frac{1}{3}\left[\frac{4c(b-4a^2)-d^2+(b+c-8a^2)(b-c)}{(b+c-8a^2)(c(b-c)-\frac{1}{2}d^2)}\right] \tag{36}$$

where a, b, c and d are given in equation (25). Also B is obtained

$$B = \left(\frac{\sqrt{N}\,\beta_{111}}{\sigma}\right)^2\left(\left(\frac{b+c}{2a}\right)^2 - \frac{8}{3}\left(\frac{b+c}{2a}\right) + \frac{28}{9}\right) \tag{37}$$

assuming

$$\beta_{111} = \beta_{222} = \beta_{112} = \beta_{122} .$$

The quantity $(b+c)/2a$ in B is equal to $(\rho_1^4 + \rho_2^4)/(\rho_1^2 + \rho_2^2)$, which is independent of α and β. Therefore, B is independent of orientations. Note that B is minimized at

$$\frac{\rho_1^4 + \rho_2^4}{\rho_1^2 + \rho_2^2} = \frac{4}{3} . \tag{38}$$

Relation (38) can be transformed into

$$(\rho_1^2 - \frac{2}{3})^2 + (\rho_2^2 - \frac{2}{3})^2 = (\frac{\sqrt{8}}{3})^2$$

which is a part of the circle with radius $\sqrt{8}/3$ and the center (2/3, 2/3) on the Cartesian plane of ρ_1^2 and ρ_2^2 as shown in Figure **2.**

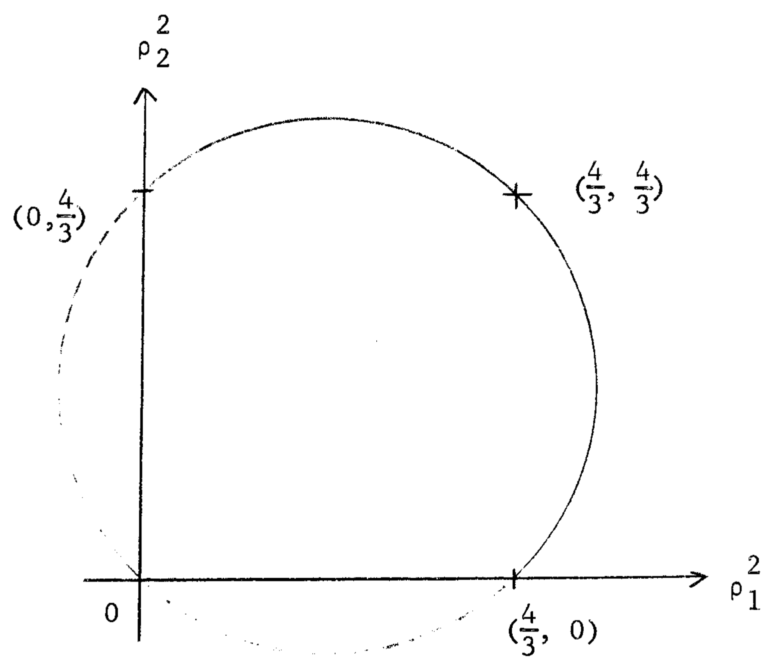


Figure 2. ρ_1 and ρ_2 for minimum B

Figure 2 shows that any combination of ρ_1 and ρ_2 which is on the solid circle line gives minimum B . The quantity, minimum B , is

$$\frac{4}{3}(\frac{\sqrt{N}\,\beta_{111}}{\sigma})^2$$

from equation (37) subject to the restriction of $\beta_{111} = \beta_{222} = \beta_{112} = \beta_{122}$.

<u>The unit circular region of interest:</u> If the region of interest is the unit circle, W_{11} is

$$W_{11} = \Omega \int_R D_1' D_1 d\underline{x} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ & 1 & 0 & 0 & 0 & 0 \\ & & 1 & 0 & 0 & 0 \\ & & & 1 & 0 & 0 \\ & & & & 1 & 0 \\ & \text{(symmetric)} & & & & \frac{1}{2} \end{bmatrix} .$$

Similary, it can be shown that

$$V = \left(\frac{1}{2a}\right) + \frac{1}{4}\left[\frac{4c(b-4a^2)-d^2+(b+c-8a^2)(b-c)}{(b+c-8a^2)(c(b-c)-\frac{1}{2}d^2)}\right]$$

and

$$B = \left(\frac{\sqrt{N}\,\beta_{111}}{\sigma}\right)^2\left[\left(\frac{b+c}{2a}\right)^2 - 2\left(\frac{b+c}{2a}\right) + \frac{5}{3}\right] .$$

In this case B is minimized at

$$\frac{b+c}{2a} = \frac{\rho_1^4 + \rho_2^4}{\rho_1^2 + \rho_2^2} = 1$$

and also independent of the angles, α and β . The combinations of ρ_1 and ρ_2 which minimize B are shown in Figure 3. The quantity, minimum B , for the unit circular region of interest is

$$\frac{2}{3}\left(\frac{\sqrt{N}\,\beta_{111}}{\sigma}\right)$$

under the assumption, $\beta_{111} = \beta_{222} = \beta_{112} = \beta_{122}$.

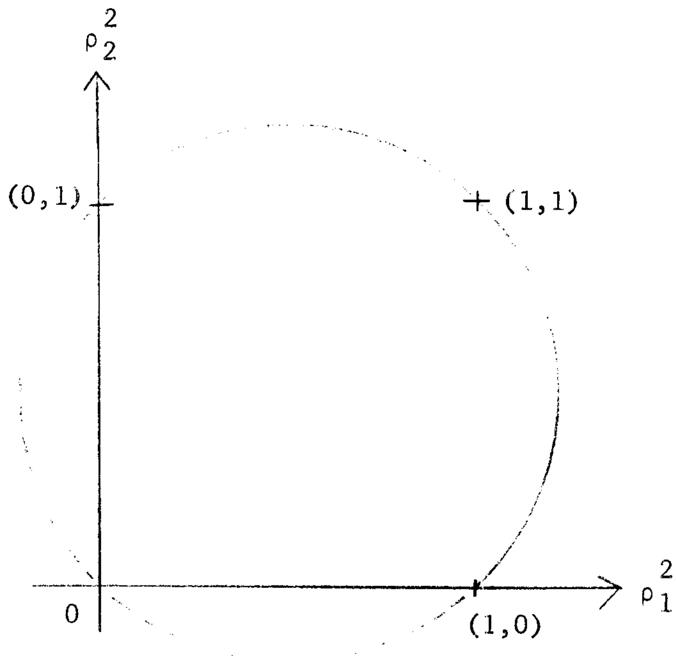


Figure 3 ρ_1 and ρ_2 for minimum B

We have discussed two particular classes of designs. Suppose one is interested in comparing the two classes of designs. The comparison could not be done completely without help of the computer. Note that, for instance, the minimization of J for the latter class of designs is difficult to accomplish analytically, since J is a function of four unknown parameters, two radii and two angles. Furthermore, if one wants to include other classes of designs for comparison, it would be very difficult. For these reasons, an optimum seeking computer program is necessary. In the next chapter, comparison of experimental designs and selection of better designs by the aid of a computer program will be discussed.

4. SELECTION OF EXPERIMENTAL DESIGNS

4.1 The Computer Program

If we are able to find an optimal design for any given number of observations, it would be very useful to an experimenter. However, it is extremely difficult to find optimal designs by the completely analytic approach. Therefore, a computer program was used to aid in the searching for optimal designs.

The computer program used in this thesis for selection of experimental designs is a modification of one used by Evans (8). The major differences from his program are the design optimality criterion and the estimator of the polynomial coefficients. Evans considered minimization of the integrated variance of estimated response $\hat{y}$ as the design criterion using the minimum bias estimator. Our design criterion is basically minimization of the integrated mean squared error of estimated slope based on the least squares estimator.

The class of designs considered for optimization is combinations of equiradial designs. Designs with points equally spaced on one, two or three circles which are concentric about the origin will be investigated to select optimal designs. Therefore, the radius of each circle and the angle of a reference design point on each circle are unknown parameters to be optimized. In this computer search for optimal designs we will restrict ourselves to the case of two independent variables (i.e., $p = 2$).

The main features of the program can be briefly sketched as follows. First, one of three criteria is chosen; V, B or J.

The shapes and sizes of the region of interest and the region of operability are selected. Then possible configurations are constructed by combining concentric circles. The program then searches for an optimal design using a simplex search, suggested by Hendrix (9), over the region of operability for the constructed configurations. The simplex search subroutine is the core part of the program. For that reason, its function is described below.

The basic search pattern used is the regular simplex in k dimensions, where k is the number of unknown parameters currently under investigation. The program anchors the original simplex at a point $\underline{a}' = (a_1, a_2, \ldots, a_k)$ in the region of operability. Using this point as one vertex, a regular simplex is formed and can be specified by the $(k + 1) \times k$ design matrix

$$D_0 = \begin{bmatrix} a_1 & a_2 & \cdot & \cdot & a_k \\ cr+a_1 & cq+a_2 & \cdot & \cdot & cq+a_k \\ cq+a_1 & cr+a_2 & \cdot & \cdot & cq+a_k \\ cq+a_1 & cq+a_2 & \cdot & \cdot & cq+a_k \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ cq+a_1 & cq+a_2 & \cdot & \cdot & cr+a_k \end{bmatrix}$$

where

$$r = \frac{1}{k\sqrt{2}}\left[(k - 1) + \sqrt{k + 1}\right],$$

$$q = \frac{1}{k\sqrt{2}}\left[\sqrt{k + 1} - 1\right]$$

and

c = a scale factor to determine the size of the simplex.

For each point represented by row d_i of D_0 a yield Y_i (V, B or J) is computed. These yields are ranked from smallest to largest. Then the rows which give poor yields are replaced by the new rows. Rules for how to drop rows of a simplex and find the new rows are explained in detail in Hendrix (9). Once the new simplex is formed, the process is repeated until it reaches an optimum. As the simplex approaches the optimum, it is reduced in size periodically by reducing the value of c. In the program $c = 0.1$ was used as the initial scale factor and reduced five times, each time by $1/10$.

4.2 Selection of Optimal and Near-Optimal Designs

The program was designed to handle any d_1 and d_2, the orders of the fitted model and the true model. However, we have exclusively searched the case of $d_1 = 2$ and $d_2 = 3$ for two independent variables. The case of $d_1 = 2$ and $d_2 = 2$ has been automatically considered, because, if the coefficients in the cubic terms of $d_2 = 3$ are assumed to be zero, this is nothing but the case of $d_1 = 2$ and $d_2 = 2$.

Two regions of interest are used; one is the unit square and the other is the unit circle. The region of operability is also divided into two types; one is limited to the region of interest and the other is not limited at all. There is obviously some practical limit or bound on the region of operability in nearly all design problems.

Therefore, the latter case should be interpreted in such a way that the region of operability is much larger than the region of interest.

Designs have been studied for observations, $6 \le N \le 12$. For $N < 6$, there are no non-singular designs. For $6 \le N \le 9$ a thorough search was conducted, but for $N \ge 10$, several good patterns obtained from $N \le 9$ were investigated. Before getting into the results of the computer search for optimal and near-optimal designs, it is important to introduce some nomenclature.

As mentioned earlier, we consider the configurations combining one, two or three concentric circles. Each configuration is described by the following way. If there are k concentric circles and n_0 center points, it is described by $n_1 - n_2 - \dots - n_k - n_0$ where n_i is the number of trials on the $i^{\underline{th}}$ circle counted from the outside circle. For example, 5-4-0 implies the configuration with five points on the outer circle, four points in the inner circle and no points at the design center. We do not consider the configurations with $n_i = 1$ for $i \ge 1$. However, there is no restriction on n_0. The best design obtained by the computer search for a given configuration is described by the notation, $(n_1,\theta_1) + (n_2,\theta_2) + \dots + (n_r,\theta_r)$, where n_j is the number of points on the $j^{\underline{th}}$ circle and θ_j is the counterclockwise rotation of a reference point on the $j^{\underline{th}}$ circle from the positive x_1-axis. Thus, the design $(6,0) + (4,\frac{\pi}{4})$ consists of two concentric n-gons. The first is a 6-gon (hexagon) centered at the origin with a point on the positive x_1-axis, and the second is a 4-gon (square) with a line connecting the reference vertex to the origin rotated counterclockwise from the x_1-axis through an angle of $\frac{\pi}{4}$ radians. This design is shown in Figure 4.

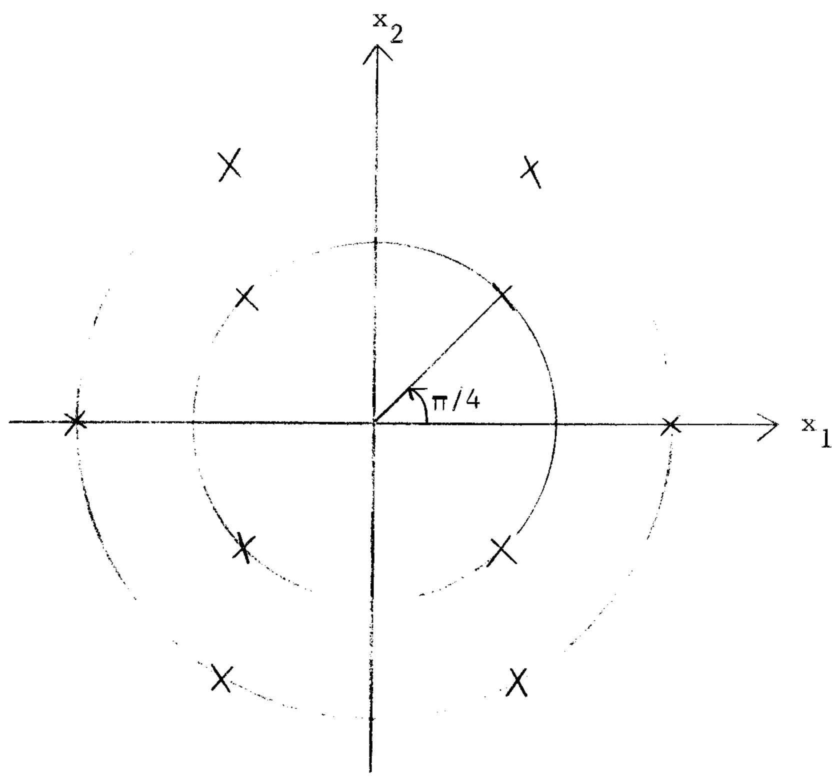


Figure 4 The design $(6,0) + (4,\frac{\pi}{4})$

The radius of the $j^{\underline{th}}$ n-gon in a design will be specified by the parameter ρ_j , while the number of trials at the origin will be denoted by N_0 . Note that N_0 could be different from n_0 .

In order to find the best design for a given N , all possible configurations should be examined and then by comparing the optimal designs obtained from each configuration, the best one is selected for the given N . For example, suppose $N = 6$. Then all possible configurations are; 5-1, 4-2, 4-2-0, 2-4-0, 3-3-0, 3-2-1, 2-3-1, and 2-2-2-0. Now the computer program finds an optimal design for each configuration, and by comparing those optimal designs, the best design for $N = 6$ is decided.

Four different cases have been considered according to the region of interest, R , and the region of operability, RO .

4.2.1 When R and RO are the Unit Square

We first consider the case where the region of operability is limited to the unit square region of interest. From the fact that one cannot realistically use the J criterion to find an optimal design without prior knowledge about β_{ijk}'s for the cubic terms, it is assumed that they are all equal. Table 6 shows the best designs found for each N when

$$\alpha = \frac{\sqrt{N}\,\beta_{111}}{\sigma} = 1 \ .$$

More than one configuration may give the best design listed in Table 6. For instance, both 4-4-2 and 4-4-2-0 give the best design for N = 10 . In Table 6 configuration which produces the best design for each N is given. The optimal and "near-optimal" designs are given in Appendix Table 7.5. If there are more than one configuration which produce a design, they are also listed in the Appendix.

An important characteristic is that every optimal design (except that of N = 6) in Table 6 contains one observation in each corner of the region of interest. For N = 6 , the possible configuration which can give one observation in each corner is 4-2-0, but this configuration supplies only singular designs. This lack of estimability helps to explain the jump in the value of J from N = 6 to N = 7 .

The optimal designs for $N \geq 9$ have the pattern of 3^2 factorial design with more than one center point in case of $N \geq 10$.

Table 6 Optimal designs when R and RO are the unit square

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B (α=1)	J
6	5-1	$(5,\frac{\pi}{20})$	1	1.012	--	--	17.568	1.428	18.996
7	4-2-1	$(4,\frac{\pi}{4})+(2,0)$	1	$\sqrt{2}$	1	--	12.541	1.611	14.152
8	4-2-2-0	$(4,\frac{\pi}{4})+(2,0)+(2,\frac{\pi}{2})$	0	$\sqrt{2}$	1	0.839	9.634	1.443	11.077
9	4-4-1	$(4,\frac{\pi}{4})+(4,0)$	1	$\sqrt{2}$	1	--	8.250	1.444	9.694
10	4-4-2	$(4,\frac{\pi}{4})+(4,0)$	2	$\sqrt{2}$	1	--	8.214	1.444	9.658
11	4-4-3	$(4,\frac{\pi}{4})+(4,0)$	3	$\sqrt{2}$	1	--	8.539	1.444	9.983
12	4-4-4	$(4,\frac{\pi}{4})+(4,0)$	4	$\sqrt{2}$	1	--	9.000	1.444	10.444

This implies that the 3^2 factorial design is recommended for a response surface second order design when R and RO are the unit square centered at the origin.

An interesting question which arises is how many points should one use in the experimental design. Since J is a measure per observation, it can be used to compare the efficiency of different designs. From Table 6, it is seen that $N = 10$ gives the best efficiency. However, the J values of $N = 9$ and $N = 11$ are close to that of $N = 11$.

Table 6 is based on $\alpha = 1$. If α is different from 1 , how does the different value of α influence the best designs and efficiency? Appendix Tables 7.1-7.4 summarize results for four different values of α .

Appendix Tables 7.1-7.4 indicate that $N = 10$ also gives the best efficiency for any α and the best configurations obtained for $\alpha = 1$ in Table 6 are left unchanged for different α's , including $\alpha = 0$ (all-variance design) and $\alpha = +\infty$ (all-bias design). Nevertheless, the best designs obtained have slightly different radii for some N according to the change of α . For instance, the best design radii for $N = 6$ remains the same for all α , but for $N = 7$ they change as α varies.

It is interesting to study the variation of the best designs by the change of α . Consider, for example, the 4-4-1 configuration of $N = 9$. Table 7 shows that the best design (all-bias design) has $\rho_1 = 1.244$ and $\rho_2 = 1$ if $\alpha = +\infty$.

Table 7 The variation of the best design of N = 9 by the change of α

α	ρ_1	ρ_2	θ_1	θ_2	V	B	J
0	$\sqrt{2}$	1	$\pi/4$	0	8.250	0	8.250
1	$\sqrt{2}$	1	$\pi/4$	0	8.250	1.444	9.694
2	$\sqrt{2}$	1	$\pi/4$	0	8.250	$\alpha^2(1.444)$	14.028
3	$\sqrt{2}$	1	$\pi/4$	0	8.250	$\alpha^2(1.444)$	21.250
$+\infty$	1.244	1	$\pi/4$	0	11.884	$\alpha^2(4/3)$	$+\infty$

In equation (38) it was shown that B is minimized at

$$\frac{\rho_1^4 + \rho_2^4}{\rho_1^2 + \rho_2^2} = \frac{4}{3}$$

which should be satisfied by the radii of the all-bias design. For $\alpha \le 3$ the best designs found are the same as that of $\alpha = 0$, the all-variance design. But as α gets large, ρ_1 approaches 1.244 while ρ_2 is left unchanged.

For the other configurations in Appendix Tables 7.1-7.4, we can construct tables similar to Table 7, which show that the best designs for each configuration are almost identical for moderate values of α.

Since Table 7 was constructed under the assumption that all β_{ijk}'s are equal (i.e., $\beta_{111} = \beta_{222} = \beta_{112} = \beta_{122}$), other ratios of β_{ijk}'s should be tested. Table 8 shows the data for three different ratios of β_{ijk}'s regarding the same 4-4-1 configuration as in Table 7.

Table 8 Variation of the best design for N = 9 for different β_{ijk}'s

β_{ijk}'s	α	ρ_1	ρ_2	θ_1	θ_2	V	B	J
$\beta_{111}:\beta_{222}:\beta_{112}:\beta_{122}$ = 1:1:0:0	0	$\sqrt{2}$	1	$\pi/4$	0	8.250	0	8.250
	1	$\sqrt{2}$	1	$\pi/4$	0	8.250	0.800	9.050
	2	$\sqrt{2}$	1	$\pi/4$	0	8.250	$\alpha^2(0.800)$	11.450
	3	$\sqrt{2}$	1	$\pi/4$	0	8.250	$\alpha^2(0.800)$	15.450
	$+\infty$	$\sqrt{2}$	1	$\pi/4$	0	8.250	$\alpha^2(0.800)$	$+\infty$
$\beta_{111}:\beta_{222}:\beta_{112}:\beta_{122}$ = $1:1:\frac{1}{3}:\frac{1}{3}$	0	$\sqrt{2}$	1	$\pi/4$	0	8.250	0	8.250
	1	$\sqrt{2}$	1	$\pi/4$	0	8.250	0.871	9.121
	2	$\sqrt{2}$	1	$\pi/4$	0	8.250	$\alpha^2(0.871)$	11.734
	3	$\sqrt{2}$	1	$\pi/4$	0	8.250	$\alpha^2(0.871)$	16.090
	$+\infty$	1.327	1	$\pi/4$	0	9.802	$\alpha^2(0.859)$	$+\infty$
$\beta_{111}:\beta_{222}:\beta_{112}:\beta_{122}$ = 1:1:3:3	0	$\sqrt{2}$	1	$\pi/4$	0	8.250	0	8.250
	1	$\sqrt{2}$	1	$\pi/4$	0	8.250	6.600	14.850
	2	1.329	1	$\pi/4$	0	9.768	$\alpha^2(5.979)$	33.685
	3	1.270	1	$\pi/4$	0	11.164	$\alpha^2(5.740)$	62.824
	$+\infty$	1.169	1	$\pi/4$	0	14.446	$\alpha^2(5.600)$	$+\infty$

In Chapter 3, slope-rotatability is recommended as a desirable property. Notice that the optimal designs for N = 6, 9, 10, 11 and 12 in Appendix Tables 7.1-7.4 are slope-rotatable. For N = 7 , an experimenter may prefer to use the slope-rotatable $(5,\frac{\pi}{20})$ design from the 5-2 configuration in Appendix Table 7.5 rather than the optimal design from the 4-2-1 configuration. Also for N = 8 , the slope-rotatable $(4,\frac{\pi}{4}) + (4,0)$ design may be used, especially since its J value is very close to that of the optimal design.

4.2.2 When R is the Unit Square and RO is Not Limited

If the region of operability is much larger than the unit square region of interest, the optimal and near-optimal designs (Appendix Table 7.6) are different from the previous case. The best designs obtained by assuming β_{ijk}'s are equal and $\alpha = 1$ are summarized in Table 9.

The best efficiency is obtained from $N = 9$, but all other N's also give J values very close to that of the optimal design. It is shown by the computer program that as long as α is not large, say $\alpha \leq 2$, the optimal configurations in Table 9 remain optimal. However, if the ratios of β_{ijk}'s are different, the optimal configurations may change. For example, if $\beta_{111}:\beta_{222}:\beta_{112}:\beta_{122} = 1:1:0:0$, then the 6-2-1 configuration replaces 5-2-2-0 as the best for $N = 9$. Nonetheless, the computer search shows that several configurations such as 6-2-1, 5-2-2-0 and 6-3-0 for $N = 9$ provide very good designs consistently for any ratios of β_{ijk}'s.

4.2.3 When R and RO are the Unit Circle

If the region of operability is identical to the unit circular region of interest, the optimal designs obtained are all equiradial designs that consists of only boundary points and center points. The best designs are shown in Table 10 and other near-optimal designs are listed in Appendix Table 7.7. Table 10 and Appendix Table 7.7 are also based on the assumption that all β_{ijk}'s are equal and $\alpha = 1$.

An important result obtained by the computer search after examining the best designs for different values of α is that the optimal designs appearing in Table 10 are α-independent. In other words, whatever the value of α is, the designs of Table 10 remain the best designs. For example, the hexagonal design of $N = 9$ is the best design for any α, which implies that the hexagonal design is the all-bias design as well as the all-variance design.

Table 9 Optimal designs when R is the unit square and RO is not limited

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	$B(\alpha=1)$	J
6	5-1	$(5,0)$	1	1.588	--	--	3.470	2.743	6.213
7	5-2-0	$(5,0)+(2,\frac{\pi}{5})$	0	1.637	0.606	--	3.264	2.600	5.864
8	5-2-1	$(5,0)+(2,\frac{\pi}{5})$	1	1.674	0.915	--	3.194	2.546	5.740
9	5-2-2-0	$(5,0)+(2,\frac{2\pi}{7})+(2,\frac{\pi}{5})$	0	1.702	0.806	0.768	3.304	2.315	5.619
10	6-2-2-0	$(6,0)+(2,\frac{2\pi}{9})+(2,\frac{\pi}{4})$	0	1.684	0.755	0.752	3.270	2.387	5.657
11	7-2-2-0	$(7,0)+(2,\frac{\pi}{4})+(2,\frac{\pi}{15})$	0	1.638	0.962	0.221	3.345	2.427	5.772
12	8-2-2-0	$(8,0)+(2,\frac{2\pi}{7})+(2,\frac{\pi}{10})$	0	1.633	0.756	0.526	3.363	2.446	5.809

Table 10 Optimal designs when R and RO are the unit circle

N	Configuration	Design	N_0	ρ	V	B (α=1)	J
6	5-1	(5,0)	1	1	14.400	0.667	15.067
7	5-2	(5,0)	2	1	13.300	0.667	13.967
8	6-2	(6,0)	2	1	13.333	0.667	14.000
9	6-3	(6,0)	3	1	13.500	0.667	14.167
10	7-3	(7,0)	3	1	13.333	0.667	14.000
11	8-3	(8,0)	3	1	13.291	0.667	13.958
12	9-3	(9,0)	3	1	13.333	0.667	14.000

For the equiradial designs, we have shown in equation (35) that

$$V = \frac{2}{\rho^2 f} + \frac{5-4f}{f(1-f)\rho^4}$$

and

$$B = \alpha^2(\rho^4 - 2\rho^2 + \frac{5}{3}) .$$

In this case when R and RO are the unit circle, $J = V + B$ is minimized at $\rho = 1$ and $f = 0.7257$ for any α and its minimum V is 13.235 and minimum B is $2\alpha^2/3$. Therefore, minimum J is 13.902 if $\alpha = 1$. In Table 10 the best efficiency is obtained from N = 11, whose J value is 13.958 and whose f is 0.727.

An important point which must be mentioned is that different ratios of β_{ijk}'s do not seem to alter the best designs in Table 10. To show this, Table 11 is constructed for N = 9. Table 11 indicates that there is no change for the best designs. Comparing Table 11 with Appendix Table 7.7, we can also notice that there is no change in the second best design.

Table 11 Three best designs for different ratios of β_{ijk}'s in case of $N = 9$

β_{ijk}'s	Configuration	Design	N_0	ρ_1	ρ_2	V	B (α=1)	J
$\beta_{111}:\beta_{222}:\beta_{112}:\beta_{122}$	6-3-0, 6-3 6-2-1, 3-3-3, 3-3-3-0	(6,0)	3	1	--	13.500	0.562	14.062
$= 1:1:0:0$	7-2-0, 7-2	(7,0)	2	1	--	13.500	0.562	14.062
	5-2-2, 5-2-2-0 2-5-2-0	(5,0)+(2,0.357)	2	1	1	14.664	0.618	15.282
$\beta_{111}:\beta_{222}:\beta_{112}:\beta_{122}$	6-3-0, 6-3 6-2-1, 3-3-3, 3-3-3-0	(6,0)	3	1	--	13.500	0.546	14.046
$= 1:1:\frac{1}{3}:\frac{1}{3}$	7-2-0, 7-2	(7,0)	2	1	--	13.500	0.546	14.046
	5-2-2, 5-2-2-0 2-5-2-0	(5,0)+(2,0.357)	2	1	1	14.664	0.570	15.234
$\beta_{111}:\beta_{222}:\beta_{112}:\beta_{122}$	6-3-0, 6-3 6-2-1, 3-3-3, 3-3-3-0	(6,0)	3	1	--	13.500	2.250	15.750
$= 1:1:3:3$	7-2-0, 7-2	(7,0)	2	1	--	13.500	2.250	15.750
	5-2-2, 5-2-2-0 2-5-2-0	(5,0)+(2,0.357)	2	1	1	14.664	2.474	17.138

Some of the reasons why the equiradial designs supply the best designs are that V is a decreasing function of ρ and B is minimized at $\rho = 1$ for any α and any ratios of β_{ijk}'s from Theorem 3. Since the region of operability is limited to the unit circle, the maximum ρ which can be achieved is 1, at which B is also minimized. Thus the equiradial designs whose boundary points on the unit circle provide the best designs. Observe that the best designs in Table 10 are all slope-rotatable.

4.2.4 When R is the Unit Circle and RO is Not Limited

In this case, exactly the same configurations appearing in Table 9 give the best designs as shown in Table 12. For near-optimal designs, see Appendix Table 7.8. The discussions for different values of α and β_{ijk}'s are quite similar to the case when R is the unit square and RO is not limited. Therefore, they are not expressed here again.

We have shown the optimal and near-optimal designs and examined their properties for four different cases according to the region of interest and the region of operability. For simplicity, let us call them Cases I, II, III, and IV in the order they have appeared previously. In other words:

Case I: When R and RO are the unit square,

Case II: When R is the unit square and RO is not limited,

Case III: When R and RO are the unit circle, and

Case IV: When R is the unit circle and RO is not limited.

Table 12 Optimal designs when R is the unit circle and RO is not limited

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B (α=1)	J
6	5-1	$(5,0)$	1	1.505	--	--	3.397	2.268	5.665
7	5-2-0	$(5,0)+(2,\frac{\pi}{5})$	0	1.555	0.591	--	3.217	2.126	5.343
8	5-2-1	$(5,0)+(2,\frac{\pi}{5})$	1	1.588	0.884	--	3.161	2.071	5.232
9	5-2-2-0	$(5,0)+(2,\frac{2\pi}{7})+(2,\frac{\pi}{5})$	0	1.621	0.782	0.752	3.241	1.870	5.111
10	6-2-2-0	$(6,0)+(2,\frac{\pi}{4})+(2,\frac{2\pi}{9})$	0	1.603	0.740	0.729	3.210	1.937	5.147
11	7-2-2-0	$(7,0)+(2,\frac{\pi}{4})+(2,\frac{\pi}{15})$	0	1.564	0.916	0.323	3.260	1.997	5.257
12	8-2-2-0	$(8,0)+(2,\frac{2\pi}{7})+(2,\frac{\pi}{10})$	0	1.575	0.840	0.435	3.163	2.117	5.280

From the data and observations we have had from 4.2.1 to 4.2.4, we can summarize the following properties regarding the optimal and near-optimal designs.

1. If ther is no limitation on the region of operability (Cases II and IV), the optimal and near-optimal designs for the unit square region of interest are very similar to those for the unit circular region of interest. This implies that the shape of region of interest is not important if limitation is not imposed on the region of operability. However, if the region of operability is limited (Cases I and III), the optimal and near-optimal designs for the unit square region of interest are quite different from those for the unit circular region of interest. Therefore, the experimenter must know what shape his region of interest is to make use of the optimal designs when the region of operability is limited.

2. The J values of the optimal and near-optimal designs of Cases II and IV are closer to each other than those of Cases I and III. This is probably due to the limited region of operability for Cases I and III.

3. For all cases, the change of α does not influence the optimal configurations as long as the values of α remain modest-sized, say $\alpha \leq 2$. Also the value of N which gives the best efficiency remains the same as α changes.

4. For all cases, there is very little change in J values due to small rotation of the inner circles of the designs obtained. Usually the change is in the fourth or fifth decimal place. Thus the angles given in the Appendices for the inner circles are not necessarily exactly optimal, but are chosen in that way, partly because it is easy to construct designs, and partly because the chosen angles are very close to the optimal angles.

5. The optimal designs have some patterns. For Case I, they follow the pattern of the 3^2 factorial design. For Case III, they are the equiradial designs which have observations on the unit circle and at the center, where the proportion of points between the circle and the center should be close to 0.7257 . Notice that the 3^2 factorial and the equiradial designs are slope-rotatable. For Cases II and IV, they follow the pattern that several points are allocated on the outside circle (more than half of observations) and a few points on the inside circle or at the center such as 5-2-1 , 6-2-2-0 , etc. These optimal designs are not slope-rotatable. Therefore, if an experimenter wants to use slope-rotatable designs for Cases II and IV, he can consult Appendix Tables 7.6 and 7.8 to select the slope-rotatable designs. For example, configuration 6-2 for $N = 8$ and configuration 5-4-0 for $N = 9$ are slope-rotatable. Since the J value of the best slope-rotatable design for each N is close to that of the best design, these slope-rotatable designs are usable in the sense of the J-criterion.

4.3 Comparison of Hexagonal, $\hat{y}$-Rotatable Central Composite and 3^2 Factorial Designs

It was shown in the previous section that the 3^2 factorial for Case I and the hexagonal for Case III are the best designs for nine observations. Another design which was introduced by Box and Wilson (6) and which has been widely used in response surface designs is the $\hat{y}$-rotatable central composite (r.c.c.) design. These three designs are slope-rotatable. We now want to investigage and compare them in more detail.

As a measure of comparison, we consider the following cirteria:

1. Minimization of J ,
2. Minimization of the rate of curvature of the variance function, and
3. Minimization of B

where criteria 2 and 3 are based on a proper standardization of the independent variables.

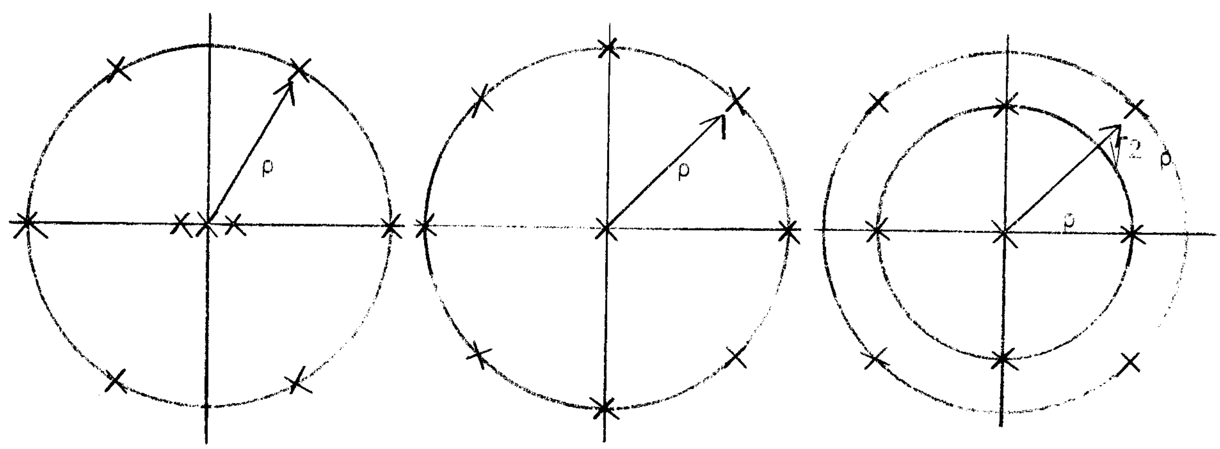
The J criterion has been used thus far as the basic criterion. Suppose all β_{ijk}'s are equal. Let α represent $\sqrt{N}\,\beta_{111}/\sigma$ as usual and let the region of interest be the unit square. The expressions for J for the designs are from Section 3.2,

$$J_{(hex)} = [\frac{3}{\rho^2} + \frac{14}{\rho^4}] + \alpha^2[\rho^4 - \frac{8}{3}\rho^2 + \frac{28}{9}] ,$$

$$J_{(r.c.c.)} = [\frac{9}{4\rho^2} + \frac{39}{2\rho^4}] + \alpha^2[\rho^4 - \frac{8}{3}\rho^2 + \frac{28}{9}] , \tag{39}$$

$$J_{(3^2)} = [\frac{3}{2\rho^2} + \frac{27}{4\rho^4}] + \frac{25}{9}\alpha^2[\rho^4 - \frac{8}{5}\rho^2 + \frac{28}{25}]$$

where ρ represents the radius which is shown in Figure 5. If the



Hexagonal Design r.c.c. Design 3^2 Factorial Design

Figure 5 The three designs

region of interest is the unit circle instead of the unit square, then they are

$$J_{(hex)} = \left[\frac{3}{\rho^2} + \frac{21}{2\rho^4}\right] + \alpha^2\left[\rho^4 - 2\rho^2 + \frac{5}{3}\right],$$

$$J_{(r.c.c.)} = \left[\frac{9}{4\rho^2} + \frac{117}{8\rho^4}\right] + \alpha^2\left[\rho^4 - 2\rho^2 + \frac{5}{3}\right], \tag{40}$$

$$J_{(3^2)} = \left[\frac{3}{2\rho^2} + \frac{81}{16\rho^4}\right] + \frac{25}{9}\alpha^2\left[\rho^4 - \frac{6}{5}\rho^2 + \frac{3}{5}\right].$$

Tables 13 through 16 are constructed in order to compare the designs by the J criterion under the four different cases described earlier.

For Cases II and IV the hexagonal design is best in terms of J values followed by the 3^2 factorial design for any value of α. However, the J values are not much different. For Case I the 3^2 factorial design is much better than the others, and the next best is the hexagonal design regardless of α. For Case III the hexagonal design is best and the $\hat{y}$-rotatable central composite design is the next best. In this case also the value of α does not influence the ranking. The 3^2 factorial design is far behind the others.

Summarizing the tables, we notice that the hexagonal design is best under three cases and the 3^2 factorial design is the best on one case, mainly because the best design is affected by the choice of the region of operability. But an important result is that the hexagonal design dominates the $\hat{y}$-rotatable central composite design for all four cases.

The <u>second</u> criterion we want to discuss for comparison is the variance function. The variance function of a second order slope-rotatable design for two independent variables is from equation (16)

$$V(\underset{\sim}{x}) = \frac{N}{2\sigma^2}\left[\mathrm{Var}(b_1) + \mathrm{Var}(b_2) + d^2(4\ \mathrm{Var}(b_{11}) + \mathrm{Var}(b_{12}))\right]$$

where $d^2 = x_1^2 + x_2^2$. Therefore, for the three designs it can be shown that the variance functions are

$$\text{hexagon:}\quad V(\underset{\sim}{x}) = \frac{3}{\rho^2} + d^2\left(\frac{21}{\rho^4}\right),$$

Table 13 Case I: R and RO are the unit square

Designs	$\alpha = 0$	$\alpha = 1$	$\alpha = 2$	$\alpha = 3$	$\alpha = +\infty$
Hexagon	$\rho=1.035$ $J=V$ $=14.987$	$\rho=1.035$ $J=14.987+1.401$ $=16.388$	$\rho=1.035$ $J=14.987+\alpha^2(1.401)$ $=20.591$	$\rho=1.035$ $J=14.987+\alpha^2(1.401)$ $=27.596$	$\rho=1.035$ $J=14.987+\alpha^2(1.401)$
R.C.C.	$\rho=1.081$ $J=V$ $=16.235$	$\rho=1.081$ $J=16.235+1.368$ $=17.593$	$\rho=1.081$ $J=16.235+\alpha^2(1.368)$ $=21.707$	$\rho=1.081$ $J=16.235+\alpha^2(1.368)$ $=28.547$	$\rho=1.081$ $J=16.235+\alpha^2(1.368)$
3^2	$\rho=1$ $J=V$ $=8.250$	$\rho=1$ $J=8.250+1.444$ $=9.694$	$\rho=1$ $J=8.250+\alpha^2(1.444)$ $=14.028$	$\rho=1$ $J=8.250+\alpha^2(1.444)$ $=21.250$	$\rho=0.894$ $J=12.422+\alpha^2(\frac{4}{3})$

Table 14 Case II: R is the unit square and RO is not limited

Designs	$\alpha = 0$	$\alpha = 1$	$\alpha = 2$	$\alpha = 3$	$\alpha = +\infty$
Hexagon	$\rho \to +\infty$ $J = V \to 0$	$\rho = 1.576$ $J = 3.471+2.663$ $= 6.134$	$\rho = 1.387$ $J = 5.336+\alpha^2(1.684)$ $= 12.070$	$\rho = 1.304$ $J = 5.508+\alpha^2(1.468)$ $= 19.820$	$\rho = 1.155$ $J = 10.125+\alpha^2(\frac{4}{3})$
R.C.C.	$\rho \to +\infty$ $J = V \to 0$	$\rho = 1.614$ $J = 3.740+2.947$ $= 6.687$	$\rho = 1.414$ $J = 6.000+\alpha^2(1.753)$ $= 13.112$	$\rho = 1.323$ $J = 7.652+\alpha^2(1.506)$ $= 21.106$	$\rho = 1.155$ $J = 12.656+\alpha^2(\frac{4}{3})$
3^2	$\rho \to +\infty$ $J = V \to 0$	$\rho = 1.249$ $J = 3.735+2.938$ $= 6.673$	$\rho = 1.095$ $J = 5.937+\alpha^2(1.777)$ $= 13.047$	$\rho = 1.025$ $J = 7.550+\alpha^2(1.506)$ $= 21.102$	$\rho = 0.894$ $J = 12.422+\alpha^2(\frac{4}{3})$

Table 15 Case III: R and RO are the unit circle

Designs	$\alpha = 0$	$\alpha = 1$	$\alpha = 2$	$\alpha = 3$	$\alpha = +\infty$
Hexagon	$\rho = 1$ $J = V$ $= 13.500$	$\rho = 1$ $J = 13.500+0.667$ $= 14.167$	$\rho = 1$ $J = 13.500+\alpha^2(0.667)$ $= 16.167$	$\rho = 1$ $J = 13.500+\alpha^2(0.667)$ $= 19.500$	$\rho = 1$ $J = 13.500+\alpha^2(\frac{2}{3})$
R.C.C.	$\rho = 1$ $J = V$ $= 16.875$	$\rho = 1$ $J = 16.875+0.667$ $= 17.542$	$\rho = 1$ $J = 16.875+\alpha^2(0.667)$ $= 19.542$	$\rho = 1$ $J = 16.875+\alpha^2(0.667)$ $= 22.875$	$\rho = 1$ $J = 16.875+\alpha^2(\frac{2}{3})$
3^2	$\rho = \frac{1}{\sqrt{2}}$ $J = V$ $= 23.250$	$\rho = \frac{1}{\sqrt{2}}$ $J = 23.250+(\frac{25}{36})$ $= 23.944$	$\rho = \frac{1}{\sqrt{2}}$ $J = 23.250+\alpha^2(\frac{25}{36})$ $= 26.028$	$\rho = \frac{1}{\sqrt{2}}$ $J = 23.250+\alpha^2(\frac{25}{36})$ $= 29.500$	$\rho = \frac{1}{\sqrt{2}}$ $J = 23.250+\alpha^2(\frac{25}{36})$

Table 16 Case IV: R is the unit circle and RO is not limited

Designs	$\alpha = 0$	$\alpha = 1$	$\alpha = 2$	$\alpha = 3$	$\alpha = +\infty$
Hexagon	$\rho \to +\infty$ $J = V \to 0$	$\rho = 1.496$ $J = 3.439+2.197$ $= 5.636$	$\rho = 1.304$ $J = 5.397+\alpha^2(1.150)$ $= 9.997$	$\rho = 1.204$ $J = 7.063+\alpha^2(0.869)$ $= 14.885$	$\rho = 1$ $J = 13.500+\alpha^2(\frac{2}{3})$
R.G.C.	$\rho \to +\infty$ $J = V \to 0$	$\rho = 1.531$ $J = 3.625+2.469$ $= 6.094$	$\rho = 1.330$ $J = 5.938+\alpha^2(1.259)$ $= 10.976$	$\rho = 1.233$ $J = 7.810+\alpha^2(0.937)$ $= 16.243$	$\rho = 1$ $J = 16.875+\alpha^2(\frac{2}{3})$
3^2	$\rho \to +\infty$ $J = V \to 0$	$\rho = 1.183$ $J = 3.651+2.442$ $= 6.093$	$\rho = 1.024$ $J = 5.911+\alpha^2(1.257)$ $= 10.936$	$\rho = 0.959$ $J = 7.549+\alpha^2(0.951)$ $= 16.104$	$\rho = 0.775$ $J = 16.562+\alpha^2(\frac{2}{3})$

$$\text{r.c.c.:} \quad V(\underset{\sim}{x}) = \frac{9}{4\rho^2} + d^2 \left(\frac{117}{4\rho^4}\right) , \tag{41}$$

$$3^2: \quad V(\underset{\sim}{x}) = \frac{3}{2\rho^2} + d^2 \left(\frac{81}{8\rho^4}\right)$$

where d is the distance of a point $\underset{\sim}{x}$ from the origin and ρ is the design radius. To compare the designs, we want to standardize the radii (subsequently the coordinates of two variables) of the designs in such a way that the integrated variances V of the three designs are all equal. The designs are then compared on the rates of curvatures of the variance functions. In other words, keeping the average V constant, we want to compare the behavior of the variance functions. Certainly, a small rate of curvature is desirable.

Suppose the region of interest is the unit square and $V = 12$ is designated. From the variance portion of equation (39) ρ should be 1.101 to accomplish $V = 12$ for the hexagonal design. The variance function for the hexagonal design is then given by

$$V(\underset{\sim}{x}) = 2.475 + 14.289\, d^2$$

in which the rate of curvature is 14.289 . Similarly, we can obtain

$$V(\underset{\sim}{x}) = 1.640 + 15.540\, d^2 \quad \text{for r.c.c.} ,$$

and

$$V(\underset{\sim}{x}) = 1.840 + 15.240\, d^2 \quad \text{for } 3^2 ,$$

where the rates of curvatures are 15.540 and 15.240 , respectively.

Therefore, at $V = 12$, the hexagonal design has the least rate of curvature. If V is different from 12 , which design has the least rate of curvature? Similar comparison was made for a number of other values of V , spanning the interval from $V = 4$ to $V = 18$. For all values checked, the hexagonal design shares the smallest rate of curvature.

The third criterion to be used to compare the designs is based on the integrated squared bias, B . We adopt the same standardization scheme employed in the second criterion. After standardization the designs are not compared on B . Suppose the region of interest is the unit square and the predetermined V is 10 . Then from equation (39) ρ should be 1.159 to accomplish $V = 10$ for the hexagonal design and subsequently B becomes $1.333\,\alpha^2$. Similarly, $\rho = 1.225$ and $B = 1.367\,\alpha^2$ for the $\hat{y}$-rotatable central composite design, and $\rho = 0.949$ and $B = 1.361\,\alpha^2$ for the 3^2 factorial design. Therefore, for the given standardization of $V = 10$, the hexagonal design is better than the $\hat{y}$-rotatable central composite design. However, the differences are quite small. In the same way Figure 6 is constructed to show how B changes for any choice of V in the range of $5 \leq V \leq 25$. We can observe that if $V < 11.2$, the order of designs from the best is the hexagonal design, the 3^2 factorial design and the r.c.c. design. If $V > 12.6$, the r.c.c. design takes the first place and the 3^2 factorial design is the second one. Nonetheless, the experimenter may, most likely, wish to standardize the designs with a reasonably small value of V . If this is the case, the conclusion is that the hexagonal design is the best one under this

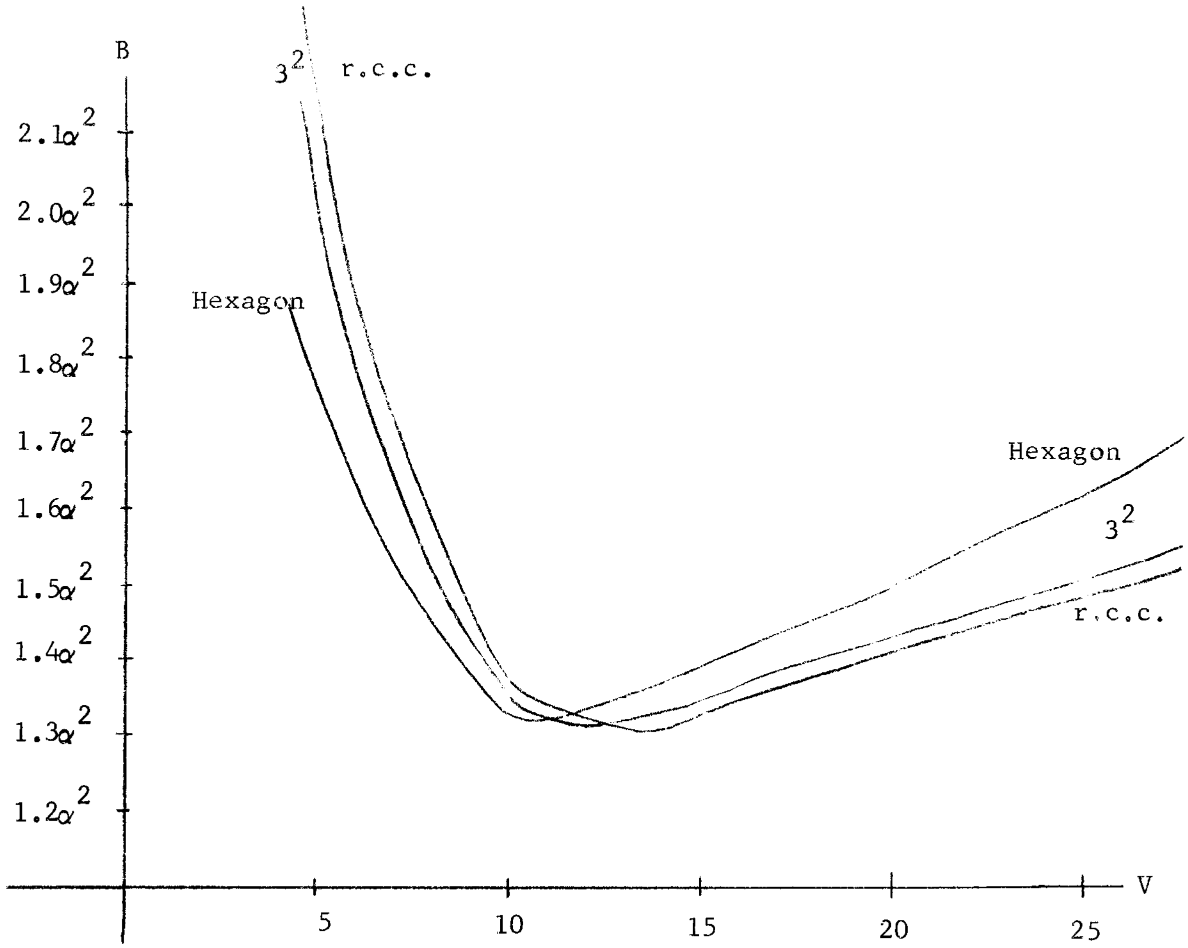


Figure 6 B as a function of V

criterion. If the region of interest is the unit circle instead of the unit square, it can be shown that similar results hold true.

We have considered three different criteria to compare the three designs. In conclusion, the hexagonal design is better than the $\hat{y}$-rotatable central composite design under any of these three criteria, and it is also better than the 3^2 factorial design except for the case when the criterion is J-minimization under the unit square region of interest and region of operability.

5. SUMMARY

This work has concerned itself with extending two main criteria to experimental designs for estimating the slope of response surfaces by second order polynomial equations when the true response is quadratic or cubic. One is the criterion of rotatability advanced by Box and Hunter (5) and the other one is the criterion of J, mean squared error integrated over a region of interest, which was introduced by Box and Draper (3,4). The least squares estimators of the polynomial coefficients were used to estimate the slope of response surfaces.

In cases where there is only one independent variable, the class of designs with three symmetric levels ($x = -h$, 0 and h, and n_1, n_0 and n_1 trials on each level, respectively) was considered. It was shown that h should be taken as large as possible to minimize V, and f^*, the optimum $f = n_1/N$, stays within a narrow range as h changes over a quite wide range. It was also observed in the case when the true model is cubic that, as $\alpha = \sqrt{N}\,\beta_3/\sigma$ increases, f^* decreases approaching 0.2847 and h^*, which minimizes J, also decreases approaching 1 .

In the case when the true response is quadratic for more than a single variable, the concept of the estimated slope variance function for an experimental design was advanced. A desirable criterion was introduced, which required the variance function to depend only on the distance from the origin of the design. Such designs insure that the estimated slope has a constant variance at all points which are the same distance from the center of the design. Designs having this property were called slope-rotatable designs. The necessary and sufficient conditions for slope-rotatability for a design were developed and the properties of slope-rotatable designs were discussed. It was shown that the class of $\hat{y}$-rotatable designs is a subset of the class of slope-rotatable designs. A number of second order slope-rotatable designs which are not $\hat{y}$-rotatable were presented and discussed.

In the case where a second order polynomial is fitted but the true model is cubic, the criterion used for optimizing designs was to minimize J , the integrated mean squared error of the estimated slope. This criterion considers not only the variance but also the bias due to the inadequacy of the fitted polynomial model. For this case two classes of designs were discussed in detail with emphasis on the integrated squared bias. One class is the set of designs whose points are equally spaced on a circle with center points, and the other is the designs of two circles with four points equally spaced on each circle.

A computer program was written to aid in the search for optimal designs under the J-criterion. Optimal and near-optimal designs in two dimensions were constructed through computer search for four different cases according to the square or circular region of interest, and the limited or unlimited region of operability. The resulting optimal and near-optimal designs were catalogued and compared. This comparison showed that when the regions of interest and operability were the unit square the optimal pattern followed the shape of 3^2 factorial design and when the regions of interest and operability were the unit circle, the optimal pattern was the design with points equally spaced on a single circle. Both optimal design patterns are slope-rotatable.

Finally, three commonly known designs for nine observations, the hexagonal design, the $\hat{y}$-rotatable central composite design and the 3^2 factorial design were compared under three different criteria. The result indicated that the hexagonal design is better than the $\hat{y}$-rotatable central composite design under all three criterion, and it is also better than the 3^2 factorial design except for one particular case, namely the unit square region of interest with design points restricted to the region.

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Appendix Table 7.1 Optimal designs when $\alpha = 0$ and the region of interest and the region of operability are the unit square

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V
6	5-1	$(5,\frac{\pi}{20})$	1	1.012	--	--	17.568
7	4-2-1	$(4,\frac{\pi}{4})+(2,0)$	1	$\sqrt{2}$	1	--	12.541
8	4-2-2-0	$(4,\frac{\pi}{4})+(2,0)+(2,\frac{\pi}{2})$	0	$\sqrt{2}$	1	0.839	9.634
9	4-4-1	$(4,\frac{\pi}{4})+(4,0)$	1	$\sqrt{2}$	1	--	8.250
10	4-4-2	$(4,\frac{\pi}{4})+(4,0)$	2	$\sqrt{2}$	1	--	8.214
11	4-4-3	$(4,\frac{\pi}{4})+(4,0)$	3	$\sqrt{2}$	1	--	8.539
12	4-4-4	$(4,\frac{\pi}{4})+(4,0)$	4	$\sqrt{2}$	1	--	9.000

Appendix Table 7.2 Optimal designs when $\alpha = 2$ and the region of interest and the region of operability are the unit square

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B	J
6	5-1	$(5,\frac{\pi}{20})$	1	1.012	--	--	17.568	$\alpha^2(1.428)$	23.280
7	4-2-1	$(4,\frac{\pi}{4})+(2,0)$	1	1.377	1	--	12.819	$\alpha^2(1.524)$	18.916
8	4-2-2-0	$(4,\frac{\pi}{4})+(2,0)+(2,\frac{\pi}{2})$	0	$\sqrt{2}$	1	0.839	9.634	$\alpha^2(1.443)$	15.406
9	4-4-1	$(4,\frac{\pi}{4})+(4,0)$	1	$\sqrt{2}$	1	--	8.250	$\alpha^2(1.444)$	14.028
10	4-4-2	$(4,\frac{\pi}{4})+(4,0)$	2	$\sqrt{2}$	1	--	8.214	$\alpha^2(1.444)$	13.992
11	4-4-3	$(4,\frac{\pi}{4})+(4,0)$	3	$\sqrt{2}$	1	--	8.539	$\alpha^2(1.444)$	14.317
12	4-4-4	$(4,\frac{\pi}{4})+(4,0)$	4	$\sqrt{2}$	1	--	9.000	$\alpha^2(1.444)$	14.778

Appendix Table 7.3 Optimal designs when $\alpha = 3$ and the region of interest and the region of operability are the unit square

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B	J
6	5-1	$(5,\frac{\pi}{20})$	1	1.012	--	--	17.568	$\alpha^2(1.428)$	30.420
7	4-2-1	$(4,\frac{\pi}{4})+(2,0)$	1	1.316	1	--	13.425	$\alpha^2(1.422)$	26.221
8	4-2-2-0	$(4,\frac{\pi}{4})+(2,0)+(2,\frac{\pi}{2})$	0	$\sqrt{2}$	1	0.839	9.634	$\alpha^2(1.443)$	22.622
9	4-4-1	$(4,\frac{\pi}{4})+(4,0)$	1	$\sqrt{2}$	1	--	8.250	$\alpha^2(1.444)$	21.250
10	4-4-2	$(4,\frac{\pi}{4})+(4,0)$	2	1.403	1	--	8.347	$\alpha^2(1.429)$	21.205
11	4-4-3	$(4,\frac{\pi}{4})+(4,0)$	3	1.395	1	--	8.750	$\alpha^2(1.418)$	21.515
12	4-4-4	$(4,\frac{\pi}{4})+(4,0)$	4	1.392	1	--	9.231	$\alpha^2(1.415)$	21.969

Appendix Table 7.4 Optimal designs when $\alpha = +\infty$ and the region of interest and the region of operability are the unit square

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B
6	5-1	$(5,\frac{\pi}{20})$	1	1.012	--	--	17.568	$\alpha^2(1.428)$
7	4-2-1	$(4,\frac{\pi}{4})+(2,0)$	1	1.183	1	--	15.751	$\alpha^2(1.340)$
8	4-2-2-0	$(4,\frac{\pi}{4})+(2,0)+(2,\frac{\pi}{2})$	0	1.258	1	0.839	15.873	$\alpha^2(1.333)$
9	4-4-1	$(4,\frac{\pi}{4})+(4,0)$	1	1.244	1	--	11.884	$\alpha^2(1.333)$
10	4-4-2	$(4,\frac{\pi}{4})+(4,0)$	2	1.244	1	--	10.852	$\alpha^2(1.333)$
11	4-4-3	$(4,\frac{\pi}{4})+(4,0)$	3	1.244	1	--	10.892	$\alpha^2(1.333)$
12	4-4-4	$(4,\frac{\pi}{4})+(4,0)$	4	1.244	1	--	11.266	$\alpha^2(1.333)$

Appendix Table 7.5 Optimal and near-optimal designs when the region of interest and the region of operability are the unit square

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B (α=1)	J
6	5-1	$(5,\frac{\pi}{20})$	1	1.012	--	--	17.568	1.428	18.996
	3-3-0	$(3,\frac{\pi}{12})+(3,\frac{5\pi}{12})$	0	1.035	0.677	--	29.278	2.075	31.354
7	4-2-1	$(4,\frac{\pi}{4})+(2,0)$	1	$\sqrt{2}$	1	--	12.541	1.611	14.152
	5-2-0 5-2	$(5,\frac{\pi}{20})$	2	1.012	--	--	16.055	1.428	17.483
	3-3-1 6-1	$(6,\frac{\pi}{12})$	1	1.035	--	--	17.072	1.402	18.474
	4-3-0	$(4,\frac{\pi}{4})+(3,0)$	0	$\sqrt{2}$	1	--	16.072	2.979	19.051
8	4-2-2-0	$(4,\frac{\pi}{4})+(2,0)+(2,\frac{\pi}{2})$	0	$\sqrt{2}$	1	0.839	9.634	1.443	11.077
	4-4-0	$(4,\frac{\pi}{4})+(4,0)$	0	$\sqrt{2}$	0.946	--	9.745	1.439	11.184
	4-2-2	$(4,\frac{\pi}{4})+(2,0)$	2	$\sqrt{2}$	1	--	11.666	1.611	13.277
	3-3-2-0 3-3-2 6-2-0 6-2	$(6,\frac{\pi}{12})$	2	1.035	--	--	14.868	1.402	16.270
	2-5-1	$(2,\frac{\pi}{4})+(5,\frac{\pi}{20})$	1	$\sqrt{2}$	1.012	--	15.898	1.414	17.312
	4-3-1	$(4,\frac{\pi}{4})+(3,0)$	1	$\sqrt{2}$	1	--	14.979	2.984	17.963

Appendix Table 7.5 (Continued)

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B (α=1)	J
	5-2-1 5-3 5-3-0	$(5,\frac{\pi}{20})$	3	1.012	--	--	16.657	1.428	18.085
9	4-4-1	$(4,\frac{\pi}{4})+(4,0)$	1	$\sqrt{2}$	1	--	8.250	1.444	9.094
	4-2-3-0	$(4,\frac{\pi}{4})+(2,0)+(3,-\frac{\pi}{17})$	0	$\sqrt{2}$	1	0.716	12.094	1.455	13.549
	4-5-0	$(4,\frac{\pi}{4})+(5,0)$	0	$\sqrt{2}$	0.995	--	12.231	1.412	13.643
	4-2-3	$(4,\frac{\pi}{4})+(2,0)$	3	$\sqrt{2}$	1	--	12.125	1.611	13.736
	2-5-2-0 2-5-2	$(2,\frac{\pi}{4})+(5,\frac{\pi}{20})$	2	$\sqrt{2}$	1.012	--	14.778	1.415	16.193
	2-6-1	$(2,\frac{\pi}{4})+(6,\frac{\pi}{12})$	1	$\sqrt{2}$	1.035	--	14.985	1.397	16.382
	6-3-0 6-3 3-3-3-0 3-3-3 6-2-1	$(6,\frac{\pi}{12})$	3	1.035	--	--	14.987	1.401	16.388
	8-1	$(8,\frac{\pi}{8})$	1	1.081	--	--	16.235	1.368	17.593
	7-2-0 7-2	$(7,\frac{\pi}{28})$	2	1.006	--	--	16.747	1.436	18.183

Appendix Table 7.6 Optimal and near-optimal designs when the region of interest is the unit square and the region of operability is not limited

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B (α=1)	J
6	5-1	(5,0)	1	1.588	--	--	3.470	2.743	6.213
	3-3-0	$(3,0)+(3,\frac{\pi}{3})$	0	1.883	1.244	--	3.465	3.439	6.904
7	5-2-0	$(5,0)+(2,\frac{\pi}{5})$	0	1.637	0.606	--	3.264	2.600	5.864
	5-2	(5,0)	2	1.575	--	--	3.407	2.646	6.053
	3-3-1	$(3,0)+(3,\frac{\pi}{3})$	1	1.732	1.422	--	3.414	2.864	6.278
	6-1	(6,0)	1	1.596	--	--	3.552	2.808	6.360
	4-2-1	$(4,0)+(2,\frac{\pi}{4})$	1	1.688	1.534	--	3.860	2.997	6.857
8	5-2-1	$(5,0)+(2,\frac{\pi}{5})$	1	1.674	0.915	--	3.194	2.546	5.740
	3-3-2-0 6-2-0	$(6,0)+(2,\frac{2\pi}{9})$	0	1.619	0.521	--	3.309	2.632	5.941
	3-3-2 6-2	(6,0)	2	1.575	--	--	3.385	2.650	6.035
	5-3-0	(5,0)+(3,0)	0	1.634	0.645	--	3.397	2.655	6.052
	5-3	(5,0)	3	1.581	--	--	3.556	2.694	6.250
	7-1	(7,0)	1	1.605	--	--	3.643	2.877	6.520
9	5-2-2-0	$(5,0)+(2,\frac{2\pi}{7})+(2,\frac{\pi}{5})$	0	1.702	0.806	0.768	3.304	2.315	5.619
	5-2-2	$(5,0)+(2,\frac{\pi}{5})$	2	1.683	1.103	--	3.219	2.537	5.756
	6-2-1	$(6,0)+(2,\frac{2\pi}{9})$	0	1.634	0.811	--	3.342	2.446	5.788
	5-4-0	(5,0)+(4,0)	0	1.678	0.802	--	3.388	2.649	6.037

Appendix Table 7.6 (Continued)

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B (α=1)	J
	3-3-3-0 6-3-0	(6,0)+(3,0)	0	1.615	0.554	--	3.389	2.651	6.040
	7-2-0	$(7,0)+(2,\frac{\pi}{15})$	0	1.581	0.167	--	3.389	2.664	6.053
	7-2	(7,0)	2	1.578	--	--	3.388	2.666	6.054
	5-3-1	(5,0)+(3,0)	1	1.659	0.863	--	3.433	2.672	6.105
	3-3-3 6-3	(6,0)	3	1.576	--	--	3.471	2.663	6.134
	4-4-1	$(4,0)+(4,\frac{\pi}{4})$	1	1.731	1.378	--	3.638	2.863	6.501
	5-4	(5,0)	4	1.592	--	--	3.755	2.776	6.531
	8-1	(8,0)	1	1.614	--	--	3.740	2.947	6.687

Appendix Table 7.7 Optimal and near-optimal designs when the region of interest and the region of operability are the unit circle

N	Configuration	Design	N_0	ρ_1	ρ_2	V	B (α=1)	J
6	5-1	(5,0)	1	1	--	14.400	0.667	15.067
	3-3-0	$(3,0)+(3,\frac{\pi}{3})$	0	1	0.643	25.955	1.048	27.003
7	5-2-0 5-2	(5,0)	2	1	--	13.300	0.667	13.967
	3-3-1 6-1	(6,0)	1	1	--	15.166	0.667	15.833
	4-2-1	$(4,0)+(2,\frac{\pi}{4})$	1	1	1	18.375	0.667	19.042
8	6-2-0 6-2 3-3-2-0 3-3-2	(6,0)	2	1	--	13.333	0.667	14.000
	5-3-0 5-3 5-2-1	(5,0)	3	1	--	13.866	0.667	14.533
	7-1	(7,0)	1	1	--	16.000	0.667	16.667
	4-2-2-0 4-2-2	$(4,0)+(2,\frac{\pi}{4})$	2	1	1	17.000	0.667	17.667
9	6-3-0 6-3 6-2-1 3-3-3-0 3-3-3	(6,0)	3	1	--	13.500	0.667	14.167

Appendix Table 7.7 (Continued)

N	Configuration	Design	N_0	ρ_1	ρ_2	V	B (α=1)	J
	7-2-0 7-2	(7,0)	2	1	--	13.500	0.667	14.167
	5-2-2-0 5-2-2 2-5-2-0	(5,0)+(2,0.883)	2	1	1	14.663	0.667	15.330
	5-4-0 5-4 5-3-1	(5,0)	4	1	--	14.850	0.667	15.517
	8-1 4-4-1	(8,0)	1	1	--	16.874	0.667	17.541

Appendix Table 7.8 Optimal and near-optimal designs when the region of interest is the unit circle and the region of operability is not limited

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B (α=1)	J
6	5-1	(5,0)	1	1.505	--	--	3.397	2.268	5.665
	3-3-0	$(3,0)+(3,\frac{\pi}{3})$	0	1.801	1.165	--	3.350	2.683	6.033
7	5-2-0	$(5,0)+(2,\frac{\pi}{5})$	0	1.555	0.591	--	3.217	2.126	5.343
	5-2	(5,0)	2	1.493	--	--	3.368	2.178	5.546
	3-3-1	$(3,0)+(3,\frac{\pi}{3})$	1	1.669	1.312	--	3.319	2.336	5.655
	6-1	(6,0)	1	1.513	--	--	3.465	2.331	5.796
	4-2-1	$(4,0)+(2,\frac{\pi}{4})$	1	1.602	1.454	--	3.746	2.523	6.269
8	5-2-1	$(5,0)+(2,\frac{\pi}{5})$	1	1.588	0.884	--	3.161	2.071	5.232
	3-3-2-0 6-2-0	$(6,0)+(2,\frac{2\pi}{9})$	0	1.538	0.513	--	3.256	2.158	5.414
	3-3-2 6-2	(6,0)	2	1.493	--	--	3.341	2.179	5.520
	5-3-0	(5,0)+(3,0)	0	1.553	0.636	--	3.351	2.185	5.536
	5-3	(5,0)	3	1.500	--	--	3.527	2.231	5.758
	7-1	(7,0)	1	1.522	--	--	3.543	2.399	5.942
9	5-2-2-0	$(5,0)+(2,\frac{2\pi}{7})+(2,\frac{\pi}{5})$	0	1.621	0.782	0.752	3.241	1.870	5.111
	5-2-2	$(5,0)+(2,\frac{\pi}{5})$	2	1.595	1.057	--	3.197	2.065	5.262
	6-2-1	$(6,0)+(2,\frac{2\pi}{9})$	1	1.566	0.805	--	3.196	2.072	5.268

Appendix Table 7.8 (Continued)

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B (α=1)	J
	5-4-0	(5,0)+(4,0)	0	1.594	0.779	--	3.341	2.181	5.522
	3-3-3-0 6-3-0	(6,0)+(3,0)	0	1.534	0.552	--	3.343	2.182	5.525
	7-2-0	(7,0)+(2,$\frac{\pi}{15}$)	0	1.500	0.160	--	3.332	2.197	5.529
	7-2	(7,0)	2	1.495	--	--	3.337	2.193	5.530
	5-3-1	(5,0)+(3,0)	1	1.576	0.845	--	3.386	2.203	5.589
	3-3-3 6-3	(6,0)	3	1.496	--	--	3.439	2.197	5.636
	4-4-1	(4,0)+(4,$\frac{\pi}{4}$)	1	1.640	1.312	--	3.543	2.387	5.930
	5-4	(5,0)	4	1.512	--	--	3.728	2.320	6.048
	8-1	(8,0)	1	1.531	--	--	3.625	2.469	6.094

Appendix 7.9 Derivation of $C\int \underline{kk}'dA = vI_p$

We want to show that $\int \underline{kk}'dA$ is a diagonal matrix whose diagonal elements are all equal. Let $\underline{k}' = (\cos\alpha_1 \; \cos\alpha_2 \; \ldots \; \cos\alpha_p)$ where

$$\sum_{i=1}^{p} \cos^2\alpha_i = 1 \; .$$

Then,

$$\underline{kk}' = \begin{bmatrix} \cos^2\alpha_1 & \cos\alpha_1\cos\alpha_2 & \cos\alpha_1\cos\alpha_3 & \cdots & \cos\alpha_1\cos\alpha_p \\ & \cos^2\alpha_2 & \cos\alpha_2\cos\alpha_3 & \cdots & \cos\alpha_2\cos\alpha_p \\ & & \cos^2\alpha_3 & \cdots & \cos\alpha_3\cos\alpha_p \\ & \text{(symmetric)} & & \ddots & \vdots \\ & & & & \cos^2\alpha_p \end{bmatrix}$$

Edwards[1/] shows that the spherical coordinates mapping is defined by

$$\begin{aligned} \cos\alpha_1 &= \cos\varphi_1 \; , \\ \cos\alpha_2 &= \sin\varphi_1 \cos\varphi_2 \; , \\ \cos\alpha_3 &= \sin\varphi_1 \sin\varphi_2 \cos\varphi_3 \; , \\ &\vdots \\ \cos\alpha_{p-2} &= \sin\varphi_1 \sin\varphi_2 \cdots \sin\varphi_{p-3} \cos\varphi_{p-2} \; , \\ \cos\alpha_{p-1} &= \sin\varphi_1 \sin\varphi_2 \cdots \sin\varphi_{p-2} \cos\theta \; , \\ \cos\alpha_p &= \sin\varphi_1 \sin\varphi_2 \cdots \sin\varphi_{p-2} \sin\theta \; , \end{aligned}$$

[1/] Edwards, C.H. 1973. Advanced Calculus of Several Variables. Academic Press, New York, New York and London, England.

and maps the interval $\varphi_i \in [0,\pi]$, $\theta \in [0,2\pi]$ onto the surface of the unit ball B^p . Edwards also shows that

$$dA = \sin^{p-2}\varphi_1 \sin^{p-3}\varphi_2 \cdots \sin^2\varphi_{p-3}\sin \varphi_{p-2}d\varphi_1 d\varphi_2 \cdots d\varphi_{p-2}d\theta \ .$$

Therefore, it can be readily shown that the off-diagonal elements of the matrix, $\int \underline{k}\underline{k}'dA$, are all zero, and the diagonal elements of the matrix are all equal, that is

$$\frac{(\sqrt{\pi})^p}{\Gamma(\frac{p+2}{2})} \ .$$

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