Designs for Estimating the Derivatives on Response Surfaces

Sung H. Park*

ABSTRACT

Criteria and designs are developed for estimating derivatives of P-variable second order polynomial response surfaces. The basic criterion used is mean square error of the estimated derivative, averaged over all directions and then averaged over a region of interest. A new design concept called slope-rotatability is introduced. A simplex search optimization program is used to find minimum mean square error designs for the two variable case for $6 \leq N \leq 12$.

1. Introduction

This paper considers design aspects of response surface experiments in which emphasis is on estimation of derivatives rather than the absolute value of the response variable. It is assumed that the response relationship is to be approximated by a low order polynomial in one or more independent variables. As usual the x's are transformations of the experimental variables, the origin of the x' coinciding with the center of some region of interest, R, over which the polynomial approximation is to be used. It is further convenient to scale so that the region R, may be described as a p-dimensional unit cube, $-1 \leq x_i \leq +1$, or as a unit sphere $\sum x_i^2 \leq 1$.

The coefficients in the polynomial are to be estimated, by the method of least squares, from observations on the response variable, $y = \eta + \varepsilon$. The observ-

* Deparment of Computer Science and Statistics, Seoul Narinal University.
This work was partially supported by the Korean Science and Engineering Foundation.

ations are taken at selected combinations of the x variables, the set of such combinations being called the experimental design. We assume the observational "errors", ε, to be independent identically distributed random variables with mean zero and variance σ^2.

Initially we will not assume that all of the design points must be confined to the region of interest.

Much of the literature on response surface analysis focuses on the variance and bias properties of $\hat{y}(x)$, the least squares estimator of $\eta(x)$. Recently Park [11], Atkinson [1], Mendenhall and Ott [9], Matteson [7], and Munsch [8] have considered design problems associated with estimation of derivatives of $\eta(x)$. In what follows we will expand the investgations of these authors to cases where the true response relationship is either quadratic or cubic in one or several x variables and is to be approximated by a second order polynomial. A new design concept, called slope-rotatability, will be introduced. However, the basic design criterion will be minimization of the average mean square error of the estimated derivative, averaged over the region of interest, R. For the case of two independent variables we have conducted an intensive investigation of designs with points equally spaced on one, two or three circles. A computer search routine has been used to find optimum designs within this class.

2. Single Independent Variable

Suppose the true model is a polynomial of degree d_2 in a single independent variable

$$\eta(x) = x_1'\beta_1 + x_2'\beta_2$$

but for one reason or another the experimenter fits a polynomial of degree $d_1 \leq d_2$,

$$\hat{y}(x) = x_1'b_1$$

where b_1 is the least squares estimate of β_1. The mean square error of the estimated slope, integrated over the region of interest is

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

Thus integrated mean square error, J, is seen to be the sum of V, the integrated variance of $d\hat{y}/dx$ and B, the integrated squared bias of $d\hat{y}/dx$.

It is well-known that the least squares estimate of β_1 is

$$b_1=(X_1'X_1)^{-1}X_1'y$$

and that $Eb_1=\beta_1+A\beta_2$ where $A=(X_1'X_1)^{-1}X_1'X_2$ is known as the alias matrix. In these relationships X_1 is the matrix of values taken by the polynomial terms in x_1 at each of the design points and similarly X_2 is the matrix of values taken by the polynomial terms in x_2 at each of the design points.

In the next three sections we will discuss designs for the following cases (i) $\hat{y}$ linear, η quadratic (ii) $\hat{y}$ quadratic, η quadratic (iii) $\hat{y}$ quadratic, η cubic.

2.1 True Model Quadratic, Linear Approximation Used

Suppose the true model is $\eta(x)=\beta_0+\beta_1x+\beta_2x^2$ but the approximation used is $\hat{y}=b_0+b_1x$. Atkinson's investigation of this case defines the region of operability within which the design points must be confined, as $-1\leq x\leq +1$. His criterion is minimization of mean square error of the estimated derivative averaged over an interval $(x_0-c,\ x_0+c)$. For two point designs with N observations the observations should be divided equally between the two points. If x_0 coincides with the center of the region of operability the two design points should be at the extremes $x=-1$ and $x=+1$. If x_0 is not at the center of the region of operability the two design points will be asymmetrically located with respect to x_0, though one point is always on the boundary of the region of operability.

In our framework we consider the independent variable to be coded and scaled so that the region of interest, R, is $-1\leq x\leq +1$. For a symmetric two point design with $N/2$ observations at $x=-h$ and $N/2$ observations at $x=+h$ it is easy to show

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

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

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

$$B=\frac{N\Omega}{\sigma^2}\int_{-1}^{1}\left[E\left(\frac{d\hat{y}}{dx}\right)-\frac{d\eta}{dx}\right]^2 dx$$

$$=\frac{N}{2\sigma^2}\int_{-1}^{1}[\beta_1-(\beta_1+2\beta_2x)]^2 dx$$

$$=\frac{4}{3}\alpha^2 \text{ where } \alpha=\frac{\sqrt{N}\beta_2}{\sigma}$$

$$J=\frac{1}{h^2}+\frac{4}{3}\alpha^2.$$

Clearly J is minimized when h is as large as feasible.

Atkinson also considers the use of three point designs and derives a condition under which the three point design is preferable.

2.2 True Model Quadratic, Quadratic Model Used

If the true model is $\eta(x)=\beta_0+\beta_1x+\beta_2x^2$ and the full model is fitted to the observations, i.e., $\hat{y}(x)=b_0+b_1x+b_2x^2$ then $B=0$ and we need consider only V. We will consider only symmetric three-point designs with n_1 observations at $x=-h$, n_0 observations at $x=0$ and n_1 observations at $x=h$, with $N=n_1+n_0+n_1$. For this design it is easy to show

$$\mathrm{Var}\left(\frac{d\hat{y}}{dx}\right)=V(b_1+2b_2x)$$

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

Integrating over the region of interest $-1\leq x\leq 1$

$$V=\frac{N\Omega}{\sigma^2}\int_{-1}^{1}\mathrm{Var}\left(\frac{d\hat{y}}{dx}\right)dx$$

$$=\frac{1}{2h^2f}+\frac{2}{3h^4f(1-2f)} \quad \text{where } f=n_1/N.$$

To minimiz V, h should be a large as feasible and once h is fixed the minimizing value of f can be obtained by setting $\frac{dV}{df}=0$. Thus

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

Table 1 shows f^* and V_{min} for a limited range of possible values of 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

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

Note f^* changes very little as h varies from 0.7 to 1.5. For $h=1$, $f^*=.2847$ which is in agreement with Atkinson's results. It should also be noted that V is not terribly sensitive to f. For example for $h=1$ and $f=f^*=.2847$, $V_{min}=7.195$; however, if $f=.25$, $V=7.333$. Thus allocation of 25% of the observations to $h=1$ and 25% to $h=-1$ is quite close to the optimal allocation. In practice, of course, since n_1 must be an integer, the optimum allocations could only be approximately achieved.

2.3 True Model Cubic, Quadratic Approximation Used

In this section we discuss the case where $\eta(x)=\beta_0+\beta_1x+\beta_2x^2+\beta_3x^3$ but the quadratic approximation $\hat{y}(x)=b_0+b_1x+b_2x^2$ is used. Again we consider only the design with n_1 observations at $x=-h$, n_0 observations at $x=0$ and n_1 observations at $x=h$. The integrated variance, V, is exactly the same as in the previous section, however, it is now necessary to evaluate the integrated squared bias, B. For the design under consideration

$$X_1'=\begin{pmatrix} 1,1,\ \cdots,\ 1,1,1,\cdots,1,1,1,\cdots,1 \\ -h,-h,\cdots,-h,0,0,\cdots,0,h,h,\cdots,h \\ h^2,h^2,\cdots,\ h^2,0,0,\cdots,0,h^2,h^2\cdots,h^2 \end{pmatrix}$$

$$X_2'=[-h^3,-h^3,\cdots,-h^3,0,,0,\cdots,0,h^3,h^3,\cdots,h^3]$$

It is easy to compute the alias matrix

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

Hence $Eb_0=\beta_0$, $Eb_1=\beta_1+h^2\beta_3$, $Eb_2=\beta_2$. Consequently the bias of the estimated slope at the point x is

$$E\left(\frac{d\hat{y}}{dx}\right)-\frac{d\eta}{dx}=E(b_1+2b_2x)-(\beta_1+2\beta_2x+3\beta_3x^2)$$
$$=h^2\beta_3-3\beta_3x^2.$$

Averaging the squared bias over the interval $-1\leq x\leq 1$

$$B=\frac{N}{2\sigma^2}\int_{-1}^{1}(h^2\beta_3-3\beta_3x^2)^2dx$$
$$=\alpha^2(h^4-2h^2+1.8) \text{ where } \alpha=\frac{\sqrt{N}\beta_3}{\sigma}.$$

Thus,

$$J=\left[\frac{1}{2h^2f}+\frac{2}{3h^4(1-2f)}\right]+\alpha^2(h^4-2h^2+1.8).$$

Since B is minimized at $h=1$ and V is a monotonically decreasing function of h, therefore J will be minimized for $1\leq h\leq\infty$ for any given α. For any fixed h one can find the minimizing value of f by setting $dJ/df=0$ which leads to exactly the same equation for f^* as given in Section 2.2. If h is limited to the region R, the optimum choice is $h^*=1$, $f^*=.2847$ for any value of α.

Table 2 shows how h^* and f^* depend on α. The values h^* and f^* were obtained by iterative calculation and were checked by substitution in the equations $\partial J/\partial f=0$. The last column of Table 2 shows values of J when h is limited to the region R, that is, for $h^*=1$ and $f^*=.2847$.

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	0.2923	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	$+\infty$	$+\infty$	$+\infty$

Table 2 : h* and f* for given α

3. Multifactor Designs

The slope of the response surface for a single variable is a scalar. However, with more than one variable the slope depends on the direction of measurement. In this section the general evaluation of J will first be developed and then, in connection with the variance of the estimated slope, the criterion of slope-rotatability will be advanced.

Suppose the true model is $\eta(x)=x_1'\beta_1+x_2'\beta_2$ and that the approximation $\hat{y}(x)=x_1'b_1$ is used, with x_1' containining the polynomial terms through order d_1 in p independent variables and x_2' containing the additional terms to bring the model up to order d_2. The notation X_1 and X_2 will be used to indicate the matrices whose rows are the values taken by x_1' and x_2' respectively at each of the design points. Also let

$$g(x)=\begin{pmatrix} \dfrac{\partial \hat{y}}{\partial x_1} \\ \vdots \\ \dfrac{\partial \hat{y}}{\partial x_p} \end{pmatrix}=D_1b_1 \quad \text{and} \quad r(x)=\begin{pmatrix} \dfrac{\partial \eta}{\partial x_1} \\ \vdots \\ \dfrac{\partial \eta}{\partial x_p} \end{pmatrix}=D_1\beta_1+D_2\beta_2$$

where D_1 and D_2 are matrices arising from the differentiation of $x_1'\beta$ and $x_2'\beta_2$ with respect to each of the p independent variables.

The estimated derivative at any point, x, in the direction specified by the $p\times 1$ vector of direction cosines, $k'=(k_1,k_2,\cdots,k_p)$ is $k'g(x)$. The mean squared error for this estimated slope is

$$J(x)=E[k'g(x)-k'r(x)]^2$$
$$=\mathrm{Var}(k'g(x))+(k's(x))'(k's(x))$$
$$=k'D_1\mathrm{Var}(b_1)D_1{}'k+s'(x)kk's(x)$$
$$=V(x)+B(x)$$

where $s(x)=Eg(x)-r(x)$ and where $V(x)$ and $B(x)$ are respectively the variance and squared bias of $k'g(x)$ at the point x. Since the direction of interest, k, is generally not specified in advance, we will next consider the average of $J(x)$ over all possible directions. The following tow lemmas are needed:

Lemma 1. The average of $V(x)$ over all possible directions is

$$\overline{V}(x)=\frac{\sigma^2}{p}\mathrm{tr}[D_1(X_1{}'X_1)^{-1}D_1{}'].$$

〈**Proof**〉 Letting $M=D_1\mathrm{Var}(b_1)D_1{}'$

$$\overline{V}(x)=\underset{k}{\mathrm{Avg}}(k'Mk)$$
$$=\underset{k}{\mathrm{Avg}}(\mathrm{tr}[k'Mk]) \text{ since } k'Mk \text{ is a scalar}$$
$$=\underset{k}{\mathrm{Avg}}(\mathrm{tr}[Mkk'])$$
$$=\mathrm{tr}[M\ \underset{k}{\mathrm{Avg}}\ (kk')].$$

It may be shown (see Appendix 1) that all of the off-diagonal elements of Avg (kk') are zero and all of the diagonal elements are equal, i.e., Aug $kk'=vI_p$. Thus

$$\overline{V}(x)=\mathrm{tr}[MvI_p]=\mathrm{tr}[vM]$$
$$=v\sum_{i=1}^{p}\lambda_i$$

where the λ_i are the eigenvalues of M. Since v is independent of M we may find v by considering the case where M is an identity matrix. Then clearly $\overline{V}(x)=1$ and since $\sum\lambda_i=p$ we must thus have $v=\frac{1}{p}$. Therefore

$$\overline{V}(x)=(1/p)\mathrm{tr}[M]=(\sigma^2/p)\mathrm{tr}[D_1(X_1{}'X_1)^{-1}D_1{}'].$$

Lemma 2. The average of $B(x)$ over all possible directions is

$$\overline{B}(x)=(1/p)s'(x)s(x).$$

〈**Proof**〉 $B(x)=\underset{k}{\text{Avg}}(s'(x)kk's(x))$

$$=s'(x)\underset{k}{\text{Avg}}(kk')s(x)$$

$$=(1/p)s'(x)s(x)$$

by the same reasoning as Lemma 1.

Combining the two lemmas we have

$$J(x)=(\sigma^2/p)\text{tr}[D_1(X_1'X_1)^{-1}D_1']+(1/p)s'(x)s(x).$$

We next wish to integrate $J(x)$ over the region of interest, R, starting with

$$V=\frac{N\Omega}{\sigma^2}\int_R \overline{V}(x)dx$$

$$=\frac{N\Omega}{p}\int_R \text{tr}[D_1(X_1'X_1)^{-1}D_1']dx$$

$$=\frac{N\Omega}{p}\int_R \text{tr}[(X_1'X_1)^{-1}D_1'D_1]dx$$

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

where $W_{11}=\Omega\int_R D_1'D_1dx$.

Next consider

$$B=\frac{N\Omega}{\sigma^2}\int_R \overline{B}(x)dx=\frac{N\Omega}{p\sigma^2}\int_R s'(x)s(x)dx.$$

Note that

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

$$=D_1Eb_1-(D_1\ \beta_1+D_2\beta_2)$$

$$=(D_1A-D_2)\beta_2.$$

Substituting for $s'(x)s(x)$ in B and carrying out the algebra and integration we may finally write

$$B=\frac{N}{p\sigma^2}\text{tr}[\beta_2\beta_2'(A'W_{11}A-2A'W_{12}+W_{22})]$$

where

$$W_{ij}=\Omega\int_R D_i'D_jdx.$$

Combining V and B we have

$$J=\frac{N}{p}\text{tr}[(X_1'X_1)^{-1}W_{11}]+\frac{N}{p\sigma^2}\text{tr}[\beta_2\beta_2'(A'W_{11}A-2A'W_{12}+W_{22})].$$

Atkinson [1] has investigated the case where the true model $\eta(x)$ is second order and a linear approximation, $\hat{y}(x)$, is used. Accordingly in the following sections we will consider only the use of second order $\hat{y}(x)$ with (i) $\eta(x)$ also second order and (ii) $\eta(x)$ third order.

3.1 Designs For Fitting Quadratic When True Model is Quadratic

If the true model is second order in p independent variables and if $\hat{y}(x)$ also contains all of the first and second order terms then there will be no bias and we need consider only the variance of the estimated derivative. From Lemma 1 of the previous section this variance averaged over all possible directions is

$$\overline{V}(x)=(\sigma_2/p)\mathrm{tr}[D(X'X)^{-1}D']$$

where now X is the matrix of values taken at the design points by the polynomial variables in the full second order equation $\hat{y}(x)$ and D is the matrix resulting from the differentiation of $\hat{y}(x)$ with respect to each of the p independent variables. In this section the subscripts on X and D are unnecessary and are deleted for convenience.

Now $\overline{V}(x)$ is, of course, still a function of $x=(x_1, x_2, \cdots, x_p)$, the point at which the derivative is being estimated. Motivated by the work of Box and Hunter [4], we now put forward a design criterion which we will call slope-rotatability. Box and Hunter sought designs for which $\mathrm{Var}(\hat{y})$ is constant on spheres around the origin in the x space. Similarly we will now consider designs such that our $\overline{V}(x)$ is a function only of the distance of x from the origin. Rotatability in the Box-Hunter sense will henceforth be called $\hat{y}$-rotatability. The following theorem gives general conditions for slope-rotatability.

Theorem 1. The ncessary and sufficient conditions for a design to be slope rotatable are

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

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

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

⟨**Proof**⟩ By straightforward but tedious algebra it may be shown that

$$\bar{V}(x)=(\sigma^2/p)\mathrm{tr}[D(X'X)^{-1}D']=(\sigma^2/p)\mathrm{tr}[X'X)^{-1}D'D]$$

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

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

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

It is immediately evident that the three conditions stated in the Theorem are sufficient to insure that $\bar{V}(x)$ is a function only of $\rho^2=\sum x_i^2$

$$\bar{V}(x)=(1/p)\sum_{i=1}^{p}\mathrm{Var}(b_i)+(1/p)[4\mathrm{Var}(b_{ii})+\sum_{\substack{j=1\\j\neq i}}^{p}\mathrm{Var}(b_{ij})]\rho^2.$$

Moreover if any of the three conditions are not satisfied then it is easy to show that there exist two points at the same distance from the origin which yield different values of $\bar{V}(x)$.

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

⟨**Proof**⟩ Box and Hunter [4] show that the covariances appearing in our conditions 1 and 2 are all zero for $\hat{y}$-rotatable designs and that furthermore $\mathrm{Var}(b_{ii})$ are equal for all i and $\mathrm{Var}(b_{ij})$ are equal for all (i,j), $i\neq j$. Thus, conditions 1, 2, and 3 are all satisfied.

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

⟨**Proof**⟩ If all odd-order moments are zero the covariance appearing in conditions 1 and 2 of the theorem are all zero, leaving only condition 3 to be satisfied.

Corollary 3. If all-order moments are zero and, in addition, all mixed fourth-order moments are equal, i.e.,

$$[i^2,j^2]=N^{-1}\sum_{k=1}^{N}x^2_{ik}x^2_{jk}$$

equal for (i,j), $i \neq j$, then the only further condition for slope-rotatability is equal $\mathrm{Var}(b_{ii})$ for all i.

〈**Proof**〉 Under the conditions stated it can be easily shown that $\mathrm{Var}(b_{ij})$ are all equal. Therefore the general conditions reduce to $\mathrm{Var}(b_{ii})$ equal for all i.

Slope-Rotatability Conditions for Case $p=2$. The special case with $p=2$ independent variables is of interest as an example and also because it will be investigated more intensively in subsequent sections. For this case the general conditions for slope-rotatability are

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

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

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

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

The last condition, of course, reduces to $\mathrm{Var}(b_{11}) = \mathrm{Var}(b_{22})$. If these conditions hold, the variance function is

$$\overline{V}(x) = \frac{1}{2\sigma^2}[\mathrm{Var}(b_1) + \mathrm{Var}(b_2)] + \frac{1}{2\sigma^2}[4\mathrm{Var}(b_{11}) + \mathrm{Var}(b_{12})]\rho^2$$

where $\rho^2 = x_1{}^2 + x_2{}^2$.

An example of a slope-rotatable design is the 3^2 factorial with each x coded to levels $-1, 0, +1$. Since all odd-order moments are zero and

$$\mathrm{Var}(b_1) = \mathrm{Var}(b_2) = \frac{\sigma^2}{6}, \quad \mathrm{Var}(b_{11}) = \mathrm{Var}(b_{22}) = \frac{\sigma^2}{2} \text{ and } \mathrm{Var}(b_{12}) = \frac{\sigma^2}{4}$$

we have

$$N\overline{V}(x) = \frac{3}{2} + \frac{81}{8}\rho^2.$$

It is of interest to note that the 3^2 factorial, though slope-rotatable, is not $\hat{y}$-rotatable.

While slope-rotatability appears to be a desirable property our basic criterion is still minimization of mean squared error averaged over some region of interest. For the case under consideration, i.e., both $\eta(x)$ and $\hat{y}(x)$ second order polynomials in p independent variables, bias is zero and we have only

$$V=\frac{N\Omega}{\sigma^2}\int_R \bar{V}(x)dx$$

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

In deriving this result we integrated $\bar{V}(x)$, the variance of the derivative at the point x averaged over all possible directions. The following theorem shows that for slope-rotatable designs and some additional easily satisfied conditions, V may be found by integrating $V_i(x)$ where $V_i(x)$ is the variance of the estimated derivative in the direction of the x_i factor axis.

Theorem 2. If (i) the design is slope-rotatable, (ii) $\mathrm{Var}(b_i)$ equal for all i and (iii) the region R is such that $\int_R x_i^p x_j^q dx=0$ for either p or q odd and $\int_R x_i^2 dx$ equal for all x_i then

$$V=\frac{N\Omega}{\sigma^2}\int_R \bar{V}(x)dx=\frac{N\Omega}{\sigma^2}\int_R V_i(x)dx.$$

⟨**Proof**⟩ The variance, $V_i(x)$, of the estimated derivative in the direction of the i^{th} factor axis is

$$V_i(x)=d_i(X'X)^{-1}d_i'\sigma^2$$

where d_i is the i^{th} row of D. By carrying out the indicated matrix multiplication we find

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

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

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

Integrating over a region, R, subject to condition (iii) of the theorem we have

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

where $a=\int_R x_i^2 dx$. From the equations for slope-rotatable designs,

$$\int_R V(x)dx = \frac{1}{p}\sum_{i=1}^{p}\mathrm{Var}(b_i) + \frac{1}{p}[4\mathrm{Var}(b_{ii}) + \sum_{\substack{j=1\\ j\neq i}}^{p}\mathrm{Var}(b_{ij})]\int_R \sum x_i^2 dx.$$

Since under the conditions of the theorem $\mathrm{Var}(b_i)$ are equal and $\int_R \sum x_i^2 dx =$ pa, it is evident that

$$\int_R \overline{V}(x)dx = \int_R V_i(x)dx.$$

Some Slope-Rotatable Designs. As indicated in Corollary 1 to Theorem 1 all $\hat{y}$-rotatable designs are also slope-rotatable, however, the converse is not true. Designs having the necessary symmetry to make

(1) all odd-order moments zero

(2) all pure second-order moments equal

(3) all pure fourth-order moments equal

(4) all mixed fourth-order moments equal

are readily seen to be slope-rotatable. This class includes central composites, three-level factorials and many other designs. In [10] a numbe of examples of two-variable slope-rotatable designs are constructed by using points equally spaced on two concentric circles. It is shown that a design with 3 equally spaced points on each of two circles plus an arbitrary number of center points is slope-rotatable. Likewise a design with 4 equally spaced points on each of two circles plus an arbitrary number of center points is slope-rotatable as are also designs with 3 or 4 points on one circle and 5 or more on a second circle. The design with 4 points on each of two circles will be singular if the 4 points on one circle have the same angular orientation with respect to the axes as do the 4 points on the second circle.

For the three-variable case, Box and Hunter [4] constructed $\hat{y}$-rotatable designs based on the icosahedron, the dodecahedron and on the cube plus octahedron (central composite design). In each case certain additional restrictions are necessary. In [10] we have shown that these same configurations are slope-rotatable even without the restrictions needed for $\hat{y}$-rotatability.

In four or more variables central composite designs with parameter $\alpha = n_c^{1/4}$, where n_c is the number of points in the "cube" part, are $\hat{y}$-rotatable. These designs are slope-rotatable for any value of α.

We have not attempted an intensive investigation of slope-rotatable designs. Instead, in the following sections, we return to considerations of possible bias from third order terms and to the basic criterion of minimization of integrated mean square error. In Section 4, we undertake an intensive investigation of twovariable designs constructed by using equally spaced points on one, two or three circles.

3.2 Quadratic Approximation-Cubic Model

In this section we consider the case where the approximating equation, $\hat{y}(x)$, is second order but the model, $\eta(x)$, is third order. We limit ourselves to the two-variable case and to two commonly used designs: (i) $n_1 \geq 6$ points equally spaced on a single circle plus n_0 center points and (ii) $n_1=4$ points on a circle of radius ρ_1, $n_2=4$ points on a second circle of radius ρ_2 and n_0 center points. These two designs include the hexagon, the 3^2 factoral and the central composite. The region over which mean square error is to be averaged will be either the unit square or the unit circle.

3.2.1 Designs With $n_1 \geq 6$ Points On Single Circle.

The design coordinates for the n_1 points on the circle of radius ρ may be represented as

$$x_{1u}=\rho \cos\left(u\frac{2\pi}{n_1}+\alpha\right)$$

$$x_{2u}=\rho \sin\left(u\frac{2\pi}{n_1}+\alpha\right)$$

with $u=0, 1, 2, \cdots, n-1$ and with α the angle between the first point and the

$$N^{-1}X_1'X_1 \begin{pmatrix} 1 & 0 & 0 & a & a & 0 \\ & a & 0 & 0 & 0 & 0 \\ & & a & 0 & 0 & 0 \\ & & & 3b & b & 0 \\ & & & & 3b & 0 \\ & & & & & b \end{pmatrix}$$

positive direction of the x_1 axis. For $\hat{y}(x)$ of the form $\hat{y}(x)=b_0+b_1x_1+b_2x_2+b_{11}x_1^2+b_{22}x_2^2+b_{12}x_1x_2$ the moment matrix $N^{-1}(X_1'X_1)$ is

with $a=\rho^2 f/2$, $b=\rho^4 f/8$, $f=n_1/N$ and $N=n_1+n_0$. Clearly this design is $\hat{y}$-rotatable as well as slope-rotatable.

Unit Square Region of Interest. If the region of interest, R, is the unit square and since the design has $\mathrm{Var}(b_1)=\mathrm{Var}(b_2)$ we may use Theorem 2 to evaluate

$$V=\frac{N\Omega}{\sigma^2}\int_{-1}^{1}\int_{-1}^{1}V\left(\frac{\partial\hat{y}}{\partial x_1}\right)dx=\frac{N}{4\sigma^2}\int_{-1}^{1}\int_{-1}^{1}\mathrm{Var}(b_1+2b_{22}x_1+b_{12}x_2)\,dx$$
$$=\frac{2}{f\rho^2}+\frac{4(5-4f)}{3f(1-f)\rho^4}.$$

The alias matrix $A=(X_1'X_1)^{-1}X_1'X_2$ is readily shown to be

$$A=\begin{pmatrix} 0 & 0 & 0 & 0\\ \frac{3}{4}\rho^2 & 0 & 0 & \frac{1}{4}\rho^2\\ 0 & \frac{3}{4}\rho^2 & \frac{1}{4}\rho^2 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 \end{pmatrix}$$

In calculating A the matrix X_2 is based on the omitted third-order terms x_1^3, x_2^3, $x_1^2x_2$, $x_1x_2^2$.

From the general expression for the integrated squared bias we have

$$B=\frac{N}{2\sigma^2}\mathrm{tr}[\beta^{2\prime}(A'W_{11}A-2A'W_{12}+W_{22})\beta_2].$$

The matrices W_{11}, W_{12}, and W_{22} are given in Appendix 2. Carrying out the indicated matrix operations we get

$$N^{-1}2\sigma^2B=(\beta^2_{111}+\beta^2_{222})\left[\left(\frac{3}{4}\rho^2-1\right)^2+\frac{4}{5}\right]$$
$$+(\beta^2_{112}+\beta^2_{122})\left[\left(\frac{1}{4}\rho^2-13\right)^2+\frac{24}{25}\right]$$
$$+6(\beta_{111}\beta_{112}+\beta_{222}\beta_{122})\left[\left(\frac{1}{4}\rho^2-\frac{1}{3}\right)^2\right].$$

It is now easy to show that B is minimized for $\rho^2=4/3$ whatever the values of the third order regression coefficients. Since V is a monotonically decreasing function of ρ, the minimum of $J=V+B$ will occur for $\rho^2 \geq 4/3$. Thus, if the design points are constrained to lie within the region of interest the $n_1 \geq 6$ points should be taken on the largest possible circle within the unit square. If the design points may be located outside of the unit square the optimum $\rho=\rho^*$ depends on the values assumed for the third order β's. Once ρ is fixed the optimum value of $f=n_1/N$ can be found by setting $dJ/df=0$ and solving to find

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

If we assume, for example, that the third order β's are equal then

$$J=\frac{3}{f\rho^2}+\frac{4(5-4f)}{3f(1-f)\rho^4}+\alpha^2\left(\rho^4-\frac{8}{3}\rho^2+\frac{28}{9}\right)$$

and Table 3 shows how ρ^* and f^* then vary with $\alpha=\sqrt{N}\beta_{111}/\sigma$. Note that ρ^* approaches $\sqrt{4/3}$ as α gets large and that f^* is relatively constant at about. 73.

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	$+\infty$	$+\infty$

Table 3 : ρ^* and f* VS. α for the unit square R

Unit Circle Region of Interest. If the region of interest, R, is the unit circle a parallel development yields

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

and

$$N^{-1}2\sigma^2B=(\beta^2_{111}+\beta^2_{222})\left[\frac{9}{16}(\rho^2-1)^2+\frac{9}{16}\right]$$
$$+(\beta^2_{112}+\beta^2_{122})\left[\frac{1}{16}(\rho^2-1)^2+\frac{11}{48}\right]$$
$$+2(\beta_{111}\beta_{122}+\beta_{222}\beta_{112})\left[\frac{3}{16}(\rho^2-1)^2-\frac{1}{16}\right].$$

The matrices W_{11}, W_{12}, W_{22} necessary for this development are given in Appendix 2.

Again it is easy to show that B is minimized for $\rho^2=1$ whatever the values of the third order β's and again since V is a monotonically decreasing function of ρ^2 the minimum of $J=V+B$ will occur for $\rho^2\geq 1$. If the design points are constrained to lie within the region of interest they should lie on the unit circle. If they may be located outside the region of interest the optimum ρ^* depends on the values of the β's. Taking $\beta_{111}=\beta_{222}=\beta_{112}=\beta_{122}$, for example, we have

$$J=\frac{2}{f\rho^2}+\frac{5-4f}{f(1-f)\rho^4}+\alpha^2(\rho^4-2\rho^2+5/3)$$

where $\alpha=\sqrt{N}\beta_{111}/\sigma$. Table 4 shows how ρ^* and f^* depend on α under this assumption.

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	$+\infty$	$+\infty$

Table 4 : ρ^* and f* VS. α for the unit circie R

In Table 4 f^* is found from

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

Note that ρ^* decreases towards $\rho^*=1$ as α increases and also note that f^* is relatively constant.

3.2.2 Designs With Points on Two Circles.

We next consider designs with 4 points equally spaced on each of two circles of radii ρ_1 and ρ_2, plus n_0 center points. Let α be the angle between the positive X_1 axis and the first point on the first circle and let β be the corresponding angle for the second circle. Then it is shown in [10] that for the

Unit Square Region of Interest.

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

and for $\beta_{111}=\beta_{222}=\beta_{112}=\beta_{122}$

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

where

$$\text{Na}=\rho_1{}^2+\rho_2{}^2$$

$$\text{Nb}=\rho_1{}^4(1+\cos^2 2\alpha)+\rho_2{}^4(1+\cos^2 2\beta)$$

$$\text{Nc}=\rho_1{}^4\sin^2 2\alpha+\rho_2{}^4\sin^2 2\beta$$

$$\text{Nd}=\rho_1{}^4\sin 4\alpha+\rho_2{}^4\sin 4\beta.$$

The ratio $(b+c)/2a$ is easily seen to be $(\rho_1{}^4+\rho_2{}^4)/(\rho_1{}^2+\rho_2{}^2)$ so that B is independent of the orientation angles α and β. Further B is minimized for

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

Unit Circle Region of Interest. It is also shown in [10] that for the unit circle region of interest

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

and for $\beta_{111}=\beta_{222}=\beta_{112}=\beta_{222}$

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

Again B is independent of the orientation angles, α and β. Also B is minimized for

$$\frac{\rho_1{}^4+\rho_2{}^4}{\rho_1{}^2+\rho_2{}^2}=1.$$

Further analytical progress appears not to be feasible. In the next section we utilize a computer search routine to find optimum designs for two independent variables.

4. Optimum Two-Variable Designs

4.1 The Computer Search Program

The computer program used in this section is based on the simplex search technique originally suggested by Spendley, Hext and Hinsworth [12], modified by Hendrix [6], and specifically tailored for optimization of design parameters by Evans [5]. In our application we consider two-variable designs consisting of points equally spaced on one, two or three circles. The parameters to be optimized are the radii of the circles and the orientation angles of the points on each circle. The objective is minimzation of integrated mean square error, J, over either the unit square or unit circle region of interest. Mean square error is computed on the assumption that the true model, $\eta(x)$, is third order but the approximation, $\hat{y}(x)$, is second order.

The basic search pattern used is the regular simplex in k dimensions where k is the number of parameters under investigation. The program anchors the original simplex at a point $a' = (a_1, a_2, \cdots, a_k)$. Using this point as one vertex, a regular simplex is formed as specified by the $(k+1)$ x k matrix D_0

$$D_0 = \begin{pmatrix} a_1 & a_2 & \cdots & a_k \\ cr+a_1 & cq+a_2 & \cdots & cq+a_k \\ cq+a_1 & cr+a_2 & \cdots & cq+a_k \\ cq+a_1 & cq+a_2 & \cdots & cq+a_k \\ \vdots & \vdots & & \vdots \\ cq+a_1 & cq+a_2 & \cdots & cr+a_k \end{pmatrix}$$

where $r = \frac{1}{k\sqrt{2}}[(k-1)+\sqrt{k+1}]$, $q = \frac{1}{k\sqrt{2}}[\sqrt{k+1}-1]$ and c is a scale factor. For each parameter combination, represented by a row of D_0, the value of J is computed. These J values are ranked and the rows of D_0 corresponding to the lowest J values are replaced by new rows according to rules given by Hendrix [6]. This procedure is repeated iteratively until the optimum is reached. As the optimum is approached the scale factor, c, is reduced periodically.

4.2 Notation For Optimum Designs

The optimization study was restricted to $6 \leq N \leq 12$. For each N all possible configurations (allocations to one, two, or three circles) were considered. The notation $n_1-n_2-n_3-n_0$ is used to denote these configurations. The first number, n_1, is always the number of points on the outermost circle and the last number is the number of center points. For example, 5—4—2 means 5 points on an outer circule, 4 points on an inner circle and 2 center points. The best design for a given configuration is denoted by $(n_1, \theta_1)+(n_2, \theta_2)+(n_3, \theta_3)$ where θ_j represents the orientation angle for the points on the j^{th} circle, i.e., the angle between the positive x_1-axis and the first point, measured counterclockwise, on that circle. Thus the design $(6, 0)+\left(4, \frac{\pi}{4}\right)$ consists of 6 points equally spaced on an outer circle starting with one point on the x_1-axis and 4 points equally spaced on an inner circle starting with one point at an angle of $\theta_2=\frac{\pi}{4}$. In the design listings the radii of the several circles are shown separately.

When the program has optimized a given configuration with respect to choice of radii and orientation angles the results are printed out. For a given N the optimum design is then found by selecting the configuration with minimum J.

4.2.1 Unit Square Region of Interest.

The designs shown in Table 5 are optimum for the case where the region of interest is the unit square and when the points are restricted to this region. Additional "near optimal" designs are given in Appendix 3. In [10] we have also found optimum designs for the case where the points are not restricted to the region of interest.

In deriving the designs of Table 5 we have assumed $\beta_{111}=\beta_{222}=\beta_{112}=\beta_{122}$ and have used $\alpha=\beta_{111}\sqrt{N}/\sigma=1$. The effect of changing these assumptions will be discussed subsequently.

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B(α=1)	J
6	5-1	$\left(5, \frac{\pi}{20}\right)$	1	1.012	—	—	17.568	1.428	18.996
7	4-2-1	$\left(4, \frac{\pi}{4}\right)+(2,0)$	1	$\sqrt{2}$	1	—	12.541	1.611	14.152
8	4-2-2-0	$\left(4, \frac{\pi}{4}\right)+(2,0)+\left(2, \frac{\pi}{2}\right)$	0	$\sqrt{2}$	1	0.839	9.634	1.443	11.077
9	4-4-1	$\left(4, \frac{\pi}{4}\right)+(4,0)$	1	$\sqrt{2}$	1	—	8.250	1.444	9.694
10	4-4-2	$\left(4, \frac{\pi}{4}\right)+(4,0)$	2	$\sqrt{2}$	1	—	8.214	1.444	9.658
11	4-4-3	$\left(4, \frac{\pi}{4}\right)+(4,0)$	3	$\sqrt{2}$	1	—	8.539	1.444	9.983
12	4-4-4	$\left(4, \frac{\pi}{4}\right)+(4,0)$	4	$\sqrt{2}$	1	—	9,000	1.444	10.444

Table 5 : Optimal designs when R and RO are the unit square

An interesting aspect of the designs of Table 5 is that for $N \geq 7$ all have one point located in each corner of the unit square and for $N \geq 9$ all designs are 3^2 factorials plus center points. Also note that for $N=6, 7,$ and 8 the designs are somewhat less efficient than those for $9 \leq N \leq 12$.

The designs of Table 5 for $9 \leq N \leq 12$ are slope-rotatable. From Appendix 3 a slope-rotatable design for $N=8$ is available with little increase in J. Slope-rotatable designs for $N=6$ and 7 involve more substantial increases in J.

Table 5 is based on $\alpha=\beta_{111}\sqrt{N}/\sigma=1$. Appendices 5. 1 to 5. 3 show optimum designs for other values of α. The tables show that the configurations based on $\alpha=1$ remain optimum for all values of α though the optimum radii undergo some change. For moderate values of α these changes are small.

A further assumption in constructing Table 5 was that $\beta_{111}=\beta_{222}=\beta_{112}=\beta_{122}$. Several other ratios of these β's were tried. These were 1 : 1 : 0 : 0, 1 : 1 : $\frac{1}{3}$: $\frac{1}{3}$ and 1 : 1 : 3 : 3. For moderate values of α the design configurations and orientation angles were unchanged; the radii changed very little.

4. 2. 2 Unit Circle Region of Interest.

The designs of Table 6 are optimum for the case where the region of interest is the unit circle and when the points are restricted to this region. Additional near-optimal designs are given in Appendix 4. In [10] we have also found designs for the case where the points are not restricted to the unit circle.

N	Configuration	Design	N_0	ρ	V	$B(\alpha=1)$	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

Table 6 : Optimal designs when R and RO are the unit circle

The most interesting aspect of Table 6 is that for all cases the designs are single circles of radius $\rho=1$. These designs are all slope-rotatable. Though the optimization was initially based on $\alpha=\beta_{111}\sqrt{N}/\sigma=1$ and $\beta_{111}=\beta_{222}=\beta_{122}=\beta_{112}$ the designs remain unchanged for any value of α and for other ratios of the third order β's. These results were anticipated in view of the analytical development of the single circle designs of Section 3. 2. 1.

For the designs presented in this section the points were restricted to the region of interest, R. In [10] we have also investigated designs not subject to this restriction. For points on one, two or three circles, the outer circle is usually only modestly outside of the Region, R, having radius between 1. 5 and 1. 8. A greater variety of configurations yield approximately equal values of J and these J values are smaller than those for the restricted case by factors of 2 or 3.

5. Summary

In this paper we have expanded the work of several other authors [1, 7, 8, 9] on design problems associated with estimation of derivatives of polynomial response functions. Our principal results relate to the use of second order polynomials. The mean squared error for the derivative in a given direction at any point, x, is averaged over all possible directions and this function of x is then averaged over a specified region of interest, R. Our basic design criterion is minimization of this averaged mean squared error. The criterion includes bias contributed by possible third order terms in the true model.

A new design concept called slope-rotatability is introduced. It requires that the variance of estimated derivation at any point x, averaged over all possible directions, be a function only of the distance of x from the center of the design. Necessary and sufficient conditions for slope-rotatability are given. These conditions are easily satisfied.

For the two-variable case a computer optimization study was conducted for a class of designs with points on one, two or three circles. The region of interest was taken to be either a unit square or a unit circle. Optimum designs, within the class considered, were found both for the case when the points were restricted to the region of interest and for the case where the points were not so restricted.

Appendix 1

To show that the off-diagonal elements of kk', averaged over all directions, are equal to zero consider

$$\int\int\cdots\int_{\sum\cos^2\theta_i=1} \cos\theta_1 \cos\theta_2 d\theta_1 d\theta_2\cdots d\theta_p.$$

Under the transformation $\alpha_i=\cos\theta_i$ this becomes

$$\int\int\cdots\int_{\sum\alpha_i^2=1} \alpha_1\alpha_2(1-\alpha_i^2)^{-1/2}d\alpha_1 d\alpha_2\cdots d\alpha_p.$$

Now for fixed values of $\alpha_3, \alpha_4, \cdots, \alpha_p$ consider the integration with rspect to α_1 and α_2

$$\int\int_C \frac{\alpha_1}{\sqrt{1-\alpha_1}} \frac{\alpha_2}{\sqrt{1-\alpha_2^2}} d\alpha_1 d\alpha_2$$

where C is the circle defined by $\alpha_1^2+\alpha_2^2=1-\alpha_3^2-\alpha_4^2-\cdots-\alpha_p^2$. Clearly the contributions along each quadrant of the circle are equal except for sign and when the signs are taken into account the integral around the full circle is zero. Since this is true for any values of $\alpha_3, \alpha_4, \cdots, \alpha_p$ the integration with respect to the α's is zero.

Appendix 2 : W_{ij} Matrices

Unit Square

$$W_{11}=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4/3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2/3 \end{pmatrix}$$

$$W_{12}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1/3 \\ 0 & 1 & 1/3 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Unit Circle

$$W_{11}=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2 \end{pmatrix}$$

$$W_{12}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 3/4 & 0 & 0 & 1/4 \\ 0 & 3/4 & 1/4 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Unit Square

$$W_{22}=\begin{pmatrix} 9/5 & 0 & 0 & 1/3 \\ 0 & 9/5 & 1/3 & 0 \\ 0 & 1/3 & 29/45 & 0 \\ 1/3 & 0 & 0 & 29/45 \end{pmatrix}$$

Unit Circle

$$W_{22}=\begin{pmatrix} 9/8 & 0 & 0 & 1/8 \\ 0 & 9/8 & 1/8 & 0 \\ 0 & 1/8 & 7/24 & 0 \\ 1/8 & 0 & 0 & 7/24 \end{pmatrix}$$

Unit Square $W_{ij}=\frac{1}{4}\int_{-1}^{1}\int_{-1}^{1} D_i' D_j dx_1 dx_2$

Unit Circle $W_{ij}=\frac{1}{\pi}\iint_{x_1^2+x_2^2\leq 1} D_i' D_j dx_1 dx_2.$

N	Design	N_0	ρ_1	ρ_2	ρ_3	V	B(α=1)	J
6	$\left(5, \frac{\pi}{20}\right)$	1	1.012	—	—	17.568	1.428	18.996
7	$\left(4, \frac{\pi}{4}\right)+(2, 0)$	1	$\sqrt{2}$	1	—	12.541	1.611	14.152
	$\left(5, \frac{\pi}{20}\right)$	2	1.012	—	—	16.055	1.428	17.483

N	Design	N_0	ρ_1	ρ_2	ρ_3	V	B	J
	$\left(6, \frac{\pi}{12}\right)$	1	1.035	—	—	17.072	1.402	18.474
8	$\left(4, \frac{\pi}{4}\right)+(2, 0)+\left(2, \frac{\pi}{2}\right)$	0	$\sqrt{2}$	1	0.839	9.634	1.443	11.077
	$\left(4, \frac{\pi}{4}\right)+(4, 0)$	0	$\sqrt{2}$	0.946	—	9.745	1.439	11.184
	$\left(6, \frac{\pi}{12}\right)$	2	1.035	—	—	14.868	1.402	16.270
9	$\left(4, \frac{\pi}{4}\right)+(4, 0)$	1	$\sqrt{2}$	1	—	8.250	1.444	9.694
	$\left(4, \frac{\pi}{4}\right)+(5, 0)$	0	$\sqrt{2}$	0.995	—	12.231	1.412	13.643
	$\left(6, \frac{\pi}{12}\right)$	3	1.035	—	—	14.987	1.401	16.388
	$\left(8, \frac{\pi}{8}\right)$	1	1.081	—	—	16.235	1.368	17.593
	$\left(7, \frac{\pi}{28}\right)$	2	1.006	—	—	16.747	1.436	18.183

Appendix 3 : Optimal and near optimal designs for R=unit square

N	Design	N_0	ρ_1	ρ_2	V	$B(\alpha=1)$	J
6	(5, 0)	1	1	—	14.400	0.667	15.067
7	(5, 0)	2	1	—	13.300	0.667	13.967
	(6, 0)	1	1	—	15.166	0.667	15.833
8	(6, 0)	2	1	—	13.333	0.667	14.000
	(5, 0)	3	1	—	13.866	0.667	14.533
	(7, 0)	1	1	—	16.000	0.667	16.667
9	(6. 0)	3	1	—	13.500	0.667	14.167
	(7, 0)	2	1	—	13.500	0.667	14.167
	(5, 0)	4	1	—	14.850	0.667	15.517
	(8, 0)	1	1	—	16.874	0.667	17.541

Appendix 4 : Optimal and near optimal designs for R=unit circle

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

Appendix 5.1 : Optimal Designs for unit spuare when $\alpha=0$

N	configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B	J
6	5-1	$\left(5, \frac{\pi}{20}\right)$	1	1.012	—	—	17.563	$\alpha^2(1.423)$	23.230
7	4-2-1	$\left(4, \frac{\pi}{4}\right)+(2,\ 0)$	1	1.377	1	—	12.819	$\alpha^2(1.524)$	18.916
8	4-2-2-0	$\left(4, \frac{\pi}{4}\right)+(2,\ 0)+\left(2, \frac{\pi}{2}\right)$	0	$\sqrt{2}$	1	0.839	9.634	$\alpha^2(1.443)$	15.406
9	4-4-1	$\left(4, \frac{\pi}{4}\right)+(4,\ 0)$	1	$\sqrt{2}$	1	—	8.250	$\alpha^2(1.444)$	14.028
10	4-4-2	$\left(4, \frac{\pi}{4}\right)+(4,\ 0)$	2	$\sqrt{2}$	1	—	8.214	$\alpha^2(1.444)$	13.992
11	4-4-3	$\left(4, \frac{\pi}{4}\right)+(4,\ 0)$	3	$\sqrt{2}$	1	—	8.539	$\alpha^2(1.444)$	14.317
12	4-4-4	$\left(4, \frac{\pi}{4}\right)+(4,\ 0)$	4	$\sqrt{2}$	1	—	9.000	$\alpha^2(1.444)$	14.773

Appendix 5.2 : Optimal Designs for unit square when $\alpha=2$

N	Configuration	Design	N_0	ρ_1	ρ_2	ρ_3	V	B	J
6	5-1	$\left(5, \frac{\pi}{20}\right)$	1	1.012	—	—	17.563	$\alpha^2(1.423)$	30.420
7	4-2-1	$\left(4, \frac{\pi}{4}\right)+(2,\ 0)$	1	1.316	1	—	13.425	$\alpha^2(1.422)$	26.221
8	4-2-2-0	$\left(4, \frac{\pi}{4}\right)+(2,\ 0)+\left(2, \frac{\pi}{2}\right)$	0	$\sqrt{2}$	1	0.839	9.634	$\alpha^2(1.443)$	22.622
9	4-4-1	$\left(4, \frac{\pi}{4}\right)+(4,\ 0)$	1	$\sqrt{2}$	1	—	8.250	$\alpha^2(1.444)$	21.250
10	4-4-2	$\left(4, \frac{\pi}{4}\right)+(4,\ 0)$	2	1.403	1	—	8.347	$\alpha^2(1.429)$	21.205
11	4-4-3	$\left(4, \frac{\pi}{4}\right)+(4,\ 0)$	3	1.395	1	—	8.750	$\alpha^2(1.418)$	21.515
12	4-4-4	$\left(4, \frac{\pi}{4}\right)+(4,\ 0)$	4	1.392	1	—	9.231	$\alpha^2(1.415)$	21.969

Appendix 5.3 : Optimal designs for unit square when $\alpha=3$

REFERENCES

[1] Atkinson, A.C. "The design of experiments to estimate the slope of a response surface", *Biometrika,* 57 1970, 319-328.

[2] Box, G.E.P. and Draper, N.R. "A basis for the selection of a response surface design", *Journal of the American Statistical Association* 54 1959, 622-654.

[3] Box, G.E.P. and Draper, N.R. "The choice of a secod order rotatable design", *Biometrika* 50, 1963, 335-352.

[4] Box, G.E.P. and Hunter, J.S. "Multi-factor experimental designs for

exploring response surfaces", *Annal of Mathemntical Statistics*. 28, 1957, 195-241.

[5] Evans, J.W. "Computer generated D-optimal, V-optimal and trace optimal minimum bias experimental designs," *Mimeograph Series,* 1974, 936, Institute of Statistics, North Carolina State University, Raleigh, North Carolina.

[6] Hendrix, C.D. "Empirical optimization in research and development," Second Gordon Research Conf. on Operations Research and Management Science. Holderness, New Hampshire (Aug. 9-13, 1971).

[7] Matteson, R.J. "Minimum bias estimation of the slope of a response surface," Unpublished M. Sc. thesis. School of Industrial and Systems Engineering, Georgia Institute of Technology, Atlanta, Georgia, 1972.

[8] Munsch, R.C. "Minimum bias designs for response surfaces. Unpublished M. Sc. thesis," School of Industial and Systems Engineering, Georgia Institute of Technology, Atlanta, Georgia, 1971.

[9] Ott, L. and Mendenhall, W. "Designs for estimating the slope of a second order linear model," *Technometrics* 14, 1972, 341-353.

[10] Park, Sung H. "Experimental Designs for Estimating the Slope of Second Order Polynomial Response Surfaces," N.C. State University Institute of Statistics Mimeograph Series 969. Dec. 1974.

[11] Park, Sung H. and Hader, R. J. "Slope-Rotatable Central Composite Designs," *Technometrics,* 4, 1978, 413-417.

[12] Spendly, W., Hext, G.R., Himsworth, F.R., "Sequential application of simplex designs in optimization and evaluationary operations," *Technometrics,* 4, 1962, 441-461.