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A Class of Multi-Factor Designs for Estimating the Slope of Response Surfaces

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ABSTRACT

A class of multi-factor designs for estimating the slope of second order response surfaces is presented. For multi-factor designs the variance of the estimated slope at a point is a function of the direction of measurement of the slope and the design. If we average the variance over all possible directions, the averaged variance is only a function of the point and the design. By choice of design, it is possible to make this variance constant for all points equidistant from the design origin. This property is called "slope-rotatability over all directions", and the necessary and sufficient conditions for a design to have this property are given and proved. The class of design with this property is mainly discussed.

KEY WORDS : Response surface designs, Slope estimation, Rotatability, Slope-rotatability

1. INTRODUCTION

This paper considers design aspects of response surface experiments in which emphasis is on estimation of derivatives rather than absolute value of the response variable η. It is assumed that the response relationship is to be approximated by the second order polynomial model in p independent variables $\underline{x}'=(x_1, x_2, \cdots, x_p)$

$$\eta(\underline{x})=\beta_0+\sum_{i=1}^{p}\beta_i x_i+\sum_{i=1}^{p}\sum_{j\geq i}^{p}\beta_{ij}x_i x_j \tag{1}$$

which may be written in matrix notation as

$$\eta(\underline{x})=\underline{x}_s'\underline{\beta} \tag{2}$$

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in which the $1 \times m$ vector $\underline{x}'_s = (1, x_1, x_2, \cdots, x_p, x_1^2, x_2^2, \cdots, x_p^2, x_1 x_2, \cdots x_{p-1} x_p)$ and $\underline{\beta}$ is the $m \times 1$ column vector of the corresponding coefficients. As usual the $x's$ are transformations of the experimental variables, the origin of the $x's$ coinciding with the center of some region of interest over which the polynomial approximation is to be used.

The coefficients in the polynomial are to be estimated, by the method of least squares, from observations on the response variable, $y_i(\underline{x}) = \eta(\underline{x}) + e_i$, where the observations are taken at n selected combinations of the x variables. The e_i are assumed to be uncorrelated random errors with zero means and constant variance, σ^2. The $\beta's$ are then estimated by least squares $\underline{b}=(X'X)^{-1}X'\underline{y}$ in which X is the $n \times m$ matrix of values of the m elements of $\underline{x}'_s$ taken at the design points and $\underline{y}$ is the $n \times 1$ matrix of y observations.

When the fitted equation $\hat{y}(\underline{x}) = \underline{x}'_s \underline{b}$, is to be used to estimate $\eta(\underline{x})$, it is well known that

$$\text{Var}\,[\hat{y}(\underline{x})] = \sigma^2 \underline{x}'_s (X'X)^{-1} \underline{x}_s. \tag{3}$$

$\text{Var}[\hat{y}(\underline{x})]$ thus depends on the particular values of the independent variables through the vector $\underline{x}'_s$. It also depends on the design through the matrix $(X'X)^{-1}$.

Much of the literature on response surface analysis has dealt with the variance and bias properties of $\hat{y}(\underline{x})$. However, some authors have focused attention on the estimation of partial derivatives of the response function with respect to the independent variables. Atkinson (1970), Murty and Studden (1972), Ott and Mendenhall (1972), Meyers and Lahoda (1975), Hader and Park (1978) and others have considered problems associated with estimation of derivatives of $\eta(\underline{x})$. In particular, Hader and Park suggested the concept of slope-rotatability, and studied slope-rotatable central composite designs.

In this paper the concept of slope-rotatability will be extended and a class of response surface designs will be discussed.

2. ESTIMATION OF DERIVATIVES

Box and Hunter (1957) suggested that, subject to a suitable scaling of the independent variables with respect to each other, it would be desirable to have equally reliable estimates of $\eta(\underline{x})$ for all points $\underline{x}' = (x_1, x_2, \cdots, x_p)$ from the origin, that is, to have the variance of $\hat{y}(\underline{x})$ be a function of $\rho = \sqrt{x_1^2 + x_2^2 + \cdots + x_p^2}$. This in turn requires $X'X$ to be invariant under rotation and therefore, designs having this property were called rotatable designs.

Suppose now that estimation of the first derivatives of $\eta(\underline{x})$ is of interest. For the second order model

$$\frac{\partial \hat{y}(\underline{x})}{\partial x_i} = b_i + 2b_{ii}x_i + \sum_{j \neq i} b_{ij}\, x_j \tag{4}$$

the variance of this derivative is a function of the point $\underline{x}$ at which the derivative is estimated, and also a function of the design through the relationship

$$\text{Var}\,(\underline{b}) = \sigma^2 (X'X)^{-1} \tag{5}$$

Hader and Park (1978) proposed an analogue of the Box-Hunter rotatability criterion, which requires that the variance of $\partial \hat{y}(\underline{x})/\partial x_i$ be constant on circles (p=2), spheres (p=3) or hyperspheres ($p \geq 4$) centered at the design origin. Estimates of the derivative over axial directions would then be equally reliable for all points $\underline{x}$ equidistant from the design origin. Hader and Park called this property as slope-rotatability, and the Box-Hunter property as $\hat{y}$-rotatability.

3. SLOPE-ROTATABILITY OVER ALL DIRECTIONS

In practice, it is often of interest to estimate the slope of the response surface at a point $\underline{x}$, not only over the axial directions, but also over any specified direction. Let

$$\underline{g}(\underline{x}) = \begin{bmatrix} \frac{\partial \hat{y}}{\partial x_1} \\ \frac{\partial \hat{y}}{\partial x_2} \\ \vdots \\ \frac{\partial \hat{y}}{\partial x_p} \end{bmatrix} = D\underline{b} \tag{6}$$

where D is the matrix arising from the differentiation of $\underline{x}_s'\underline{b}$ with respect to each of the p independent variables. The estimated derivative at any point $\underline{x}$ in the direction specified by the $p \times 1$ vector of direction cosines

$$\underline{k}' = (k_1, k_2, \cdots, k_p) \tag{7}$$

is $\underline{k}'\underline{g}(\underline{x})$ where $\sum_{i=1}^{p} k_i^2 = 1$. The variance of this slope is

$$V(\underline{x}) = \text{Var}\,[\underline{k}'\underline{g}(\underline{x})] = \underline{k}' D\, \text{Var}\,(\underline{b})\; D'\underline{k} = \sigma^2 \underline{k}' D\,(X'X)^{-1} D'\underline{k} \tag{8}$$

If we are interested in all possible directions of $\underline{k}$, we want to consider the average of $V(\underline{x})$ over all possible directions. The following lemma is needed.

Lemma : The average of $V(\underline{x})$ over all possible directions is

$$\bar{V}(\underline{x}) = \frac{\sigma^2}{p}\, \text{tr}\,[D\,(X'X)^{-1} D']. \tag{9}$$

(Proof) Letting $M = D\, \text{Var}\,(\underline{b})\; D'$

$$\bar{V}(\underline{x}) = \underset{\underline{k}}{\text{Avg}}\,(\underline{k}' M\underline{k}) = \underset{\underline{k}}{\text{Avg}}\,(\text{tr}\,[\underline{k}' M k]) \quad \text{since } \underline{k}' M\underline{k} \text{ is a scalar.}$$

$$= \underset{\underline{k}}{\text{Avg}}\,(\text{tr}\,[M\underline{k}\underline{k}']) = \text{tr}\,[M\; \underset{\underline{k}}{\text{Avg}}\,(\underline{k}\underline{k}')].$$

It may be shown (see Appendix) that all of the off-diagonal elements of Avg($\underline{k}\underline{k}'$) are zero and all of the diagonal elements are equal, i.e., $\text{Avg}(\underline{k}\underline{k}') = \nu I_p$. Thus

$$\bar{V}(\underline{x}) = \text{tr}\,[M\nu I_p] = \text{tr}\,[\nu M] = \nu \sum_{i=1}^{p} \lambda_i$$

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

$$\bar{V}(\underline{x}) = (1/p)\,\text{tr}\,[M] = (\sigma^2/p)\,\text{tr}\,[D(X'X)^{-1}D'].$$

Note that $\bar{V}(\underline{x})$ is a function of $\underline{x}$, the point at which the derivative is being estimated, and also a function of the design. By choice of design it is possible to make this variance $\bar{V}(\underline{x})$ constant for all points equidistant from the design origin. This property will henceforth be called "Slope-rotatability over all directions". In this sense, the slope-rotatability by Hader and Park may be called "slope-rotatability over axial directions". The following theorem gives general conditions for a design to be slope-rotatable over all directions.

Theorem : The necessary and sufficient conditions for a design to be slope-rotatable over all directions are

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

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

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

(Proof) By straightforward but tedious algebra it may be shown that

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

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

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

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

It is immediately evident that the three conditions stated in the theorem are sufficient to insure that

$\bar{V}(\underline{x})$ is a function only of $\rho^2 = \sum x_i^2$

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

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 $\bar{V}(\underline{x})$.

Corollary 1 : All $\hat{y}$-rotatable designs in the Box-Hunter sense are slope-rotatable over al directions.
(Proof) Box and Hunter (1957) show that the covariances appearing in our conditions 1 and 2 are all zero for $\hat{y}$-rotatable designs and that furthermore Var(b_{ii}) are equal for all i and 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-rotatable over all directions.
(Proof) If all odd-order moments are zero the covariance appearing in conditions 1 and 2 of the theorem are all zero, leading 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.,

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

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

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

4. CASE OF TWO INDEPENDENT VARIABLES

For the special case with $p = 2$ independent variables, the necessary and sufficient conditions for slope-rotatability over all directions are

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

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

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

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

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

$$\bar{V}(\underline{x}) = \frac{1}{2\sigma^2}\left[\text{Var}(b_1) + \text{Var}(b_2)\right] + \frac{1}{2\sigma^2}\left[4\,\text{Var}(b_{11}) + \text{Var}(b_{12})\right]\rho^2$$

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

An example of the class of slope-rotatable designs over all directions is the 3^2 factorial design of 9 design points with each x coded to levels -1, 0, 1. Since all odd-order moments are zero and

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

we have

$$n\bar{V}(\underline{x}) = \frac{3}{2} + \frac{81}{8}\rho^2.$$

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

5. CLASS OF SLOPE-ROTATABLE DESIGNS OVER ALL DIRECTIONS

As mentioned in Corollary 1, all $\hat{y}$-rotatable designs are also slope-rotatable over all directions. 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 over all directions. This class includes central composites, three-level factorials and many other designs. The central composite designs which are slope-rotatable over axis directions in Hader and Park (1978) are slope-rotatable over all directions.

It can be 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.

For the three-variable case, Box and Hunter (1957) 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. We can show that these same configurations are slope-rotatable over all directions 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 over all directions for any value of α.

6. CONCLUDING REMARKS

In this paper we have considered design problems associated with estimation of derivatives of second order polynomial response functions. The variance of the derivative $V(\underline{x})$ in the equation (8) at any point $\underline{x}$ is a function of direction and a function of design. If $V(\underline{x})$ is averaged over all directions, the averaged variance $\bar{V}(\underline{x})$ is only a function of the point $\underline{x}$ and the design. By choice of design, it is possible to make $\bar{V}(\underline{x})$ constant for all points equidistant from the design origin. The class of design with such property was called slope-rotatable over all directions. Necessary and sufficient conditions to be this class of designs were given, and several designs in this class of designs were illustrated.

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(Appendix)

To show that the off-diagonal elements of $\underline{k}\underline{k}'$, averaged over all directions, are equal to zero consider

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

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

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

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

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

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.

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