Journal of Statistics Applications & Probability
An International Journal

http://dx.doi.org/10.12785/jsap/040303

On Slope Estimation Capabilities of Some Second Order Response Surface Designs

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Received: 5 May 2015, Revised: 3 Oct. 2015, Accepted: 18 Oct. 2015
Published online: 1 Nov. 2015

Abstract: Two second order response surface designs (central composite design and extended central composite design) are compared on the basis of their slope estimation capabilities of a response function using quantile plots. A large number of points is randomly generated on a sphere of radius centred at the origin in a given region of interest. The scaled average slope variance is evaluated at each of these points and the quantiles of the resulting values are plotted. Both designs were compared using slope rotatability design criterion and result obtained show that both designs have stable slope variance and the extended central composite design is better than the central composite design for large values of the radius.

Keywords: Extended central composite design, Central composite design, Quantile plots, Scaled average slope variance, Slope rotatability

1 Introduction

Response surface methodology comprises a collection of mathematical and statistical techniques for empirical modelling and analysis of problems in which a response of interest is influenced by several variables; (see Box and Draper [3] and Montgomery [13]). The major goals in using response surface methodology are finding a suitable approximating function for the purpose of predicting future response and determining what value of the independent variables are optimum as far as the response is concerned. The central composite design (CCD) proposed by Box and Wilson [5] allows for estimation of all the parameters in a full second order model and possesses good statistical properties such as orthogonality, rotatability, slope rotatability etc. Kim [10] extended the CCD by using two numbers to indicate the axial point and studied some of its properties. Studies on the extended CCD (ECCD) reveal that it has more statistical properties than the Box and Wilson CCD. For instance the ECCD possess exact uniform precision while the CCD have near uniform precision. The ECCD also have other statistical properties like rotatability, slope rotatability, both orthogonality and rotatability, rotatability and uniform precision, orthogonality and slope rotatability. In addition, Park and Park [16] compared Box and Wilson CCD and the extended CCD on the basis of uniform precision and concluded that the ECCD performs better than the CCD.

However, it is more convenient to compare competing designs that equally have same statistical property. Both the CCD and the extended CCD possess the slope rotatability criterion, therefore, we shall compare both designs on the basis of their slope estimation capabilities using quantile plots. The use of quantile plots to describe the distribution of the predicted variances on a given sphere and compare some response surface designs was proposed by Khuri, Kim and Um [9]. A graphical method for evaluating the slope estimation capability of a given response surface design as shown by Jang and Park [8] involves the use of slope variance dispersion graph, an analogue of the variance dispersion graph to compare designs on the basis of their slope estimation capabilities. It was observed that the slope variance dispersion graph considered only maximum and minimum values of the scaled average slope variance (SASV) and does not give information about the actual distribution of the scaled average slope variance on the hypersphere. In an effort to provide more information concerning the SASV, the scaled average slope variance quantile (SASVQ) plots was proposed for

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describing the distribution of the SASV on a hypersphere inside a region of interest using quantile plots. The SASVQ plots was also used to compare some response surface designs (CCD, Box-Behnken, Hoke and Roquemore designs). Knowledge of the quantile values of the SASV will give such useful information as the first quartile, median, third quartile and so on about the distribution of a given design (see Kim, Um and Khuri [12]). In this work, we shall use the SASVQ plots to compare the SASV of the CCD and ECCD.

In response surface design, difference between the estimated responses at two points is usually of greater interest than the response at individual locations. Estimation of local slope (that is rate of change) of the response is of interest when differences at two points are involved. For instance, interest can be in the estimation of the rate of change in the yield of a crop to various fertilizer or herbicide doses, or in the rate of chemical reaction. The research in designs for estimating slope was initiated by Atkinson [1]. Many other works have been done in slope estimation; see for example, Ott and Mendenhall [14], Hader and Park [7], Park [15] and Ying, Pukelsheim and Draper [17]. When interest is in estimating the slope of a response surface, slope rotatability is a desirable criterion. Hader and Park [7] introduced slope rotatability as an analogue of Box and Hunter [4] rotatability, which is referred as slope rotatability over axial direction. Slope rotatability over axial direction was extended to slope rotatability over all direction by Park [15].

2 Preliminaries

2A Scaled Average Slope Variance

Consider a $p-$ parameter second order model in k variables of interest(factors), $x_1, x_2, \ldots, x_k$

$$y(x) = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j + e \tag{1}$$

which can be written in matrix notation as

$$y(\underline{x}) = f'(\underline{x})\beta \tag{2}$$

where $\underline{x} = x_1, x_2, \ldots, x_k$, $f'(\underline{x}) = (1, x_1, x_2, \ldots, x_k, x_1^2, x_2^2, \ldots, x_k^2, x_1x_2, x_1x_3, \ldots, x_{k-1}x_k)$and β is an $p \times 1$ vector of constant coefficients, e is assumed to be uncorrelated random errors with zero mean and constant variance,σ^2. The fitted model of (1) can be expressed as

$$\hat{y}(x) = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i + \sum_{i=1}^{k} \hat{\beta}_{ii} x_i^2 + \sum_{i<j}\sum \hat{\beta}_{ij} x_i x_j \tag{3}$$

or in matrix notation as

$$\hat{y}(\underline{x}) = f'(\underline{x})\hat{\beta} \tag{4}$$

The least square estimator of β is given by

$$\hat{\beta} = (X'X)^{-1}X'y \tag{5}$$

X is an $N \times p$ matrix of rank p and y is the $N \times 1$vector of response values.

Suppose, interest is in the estimation of the first order partial derivative of $\hat{y}$ with respect to each of the independent variables of interest $x_1, x_2, \ldots, x_k$, that is

$$\frac{\delta \hat{y}(x)}{\delta x_i} = \hat{\beta}_i + 2\hat{\beta}_{ii} x_i + \sum_{j \neq i} \hat{\beta}_{ij} x_j \tag{6}$$

The variance of(6)is a function of the point $(x_1, x_2, \ldots, x_k)$ and also a function of the design through this relationship

$$Var(\hat{\beta}) = (X'X)^{-1}\sigma^2 \tag{7}$$

Slope rotatability over axial direction requires that the variance of $\frac{\delta \hat{y}(x)}{\delta x_i}$ be a constant on circles, spheres or hyperspheres centred at the origin of the design. Then estimates of the first order derivative would have equal precision at all points $(x_1, x_2, \ldots, x_k)$ equidistant from the design origin. The criterion is called slope rotatability over axial direction.

Sometimes, interest might be in the estimation of the slope of the response surface not only on the axial direction but also at any specified direction of the x_i. This is referred to slope rotatability over all direction.

Let $g(\underline{x})$ be a vector of $\hat{y}(x)$

$$g(\underline{x}) = \begin{bmatrix} \frac{\delta \hat{y}(x)}{\delta x_1} \\ \frac{\delta \hat{y}(x)}{\delta x_2} \\ \vdots \\ \frac{\delta \hat{y}(x)}{\delta x_k} \end{bmatrix} = J' \underline{\hat{\beta}} \tag{8}$$

where $J = [0, I_k, 2diag(x_1, x_2, \ldots, x_k), J^*]$ is a $k \times p$ matrix arising from differentiating $\hat{y}(x)$

$$J^* = \begin{bmatrix} x_2 & x_3 & \ldots & x_k & 0 & 0 & \ldots & 0 & 0 & 0 & \ldots & 0 & \ldots & 0 & 0 & 0 \\ x_1 & 0 & \ldots & 0 & x_3 & x_4 & \ldots & x_k & 0 & 0 & \ldots & 0 & \ldots & 0 & 0 & 0 \\ 0 & x_1 & \ldots & 0 & x_2 & 0 & \ldots & 0 & x_4 & x_5 & \ldots & x_k & \ldots & 0 & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & x_1 & 0 & 0 & \ldots & x_2 & 0 & 0 & \ldots & x_3 & \ldots & 0 & x_{k-2} & x_{k-1} \end{bmatrix}$$

The estimated derivative of $\hat{y}(x)$at any point $\underline{x}$ in the direction specified by the unit vector $\underline{w} = (w_1, w_2, \ldots, w_k)'$ is defined as $w'g(\underline{x})$

where $\sum_{i=1}^{k} w_i^2 = 1$

This slope variance is

$$\begin{aligned} V(\underline{x}) &= Var\left[\underline{w}'g(\underline{x})\right] \\ &= \underline{w}'JVar(\hat{\beta})J'\underline{w} \\ &= \sigma^2 \underline{w}'J(X'X)^{-1}J'w \end{aligned} \tag{9}$$

If interest is in all possible directions of $\underline{w}$ then we consider the average of $V(\underline{x})$ over all possible direction. This is called the average slope variance, $\overline{V}(\underline{x})$.

$$\overline{V}(\underline{x}) = \frac{\sigma^2}{k}\left[J(X'X)^{-1}J'\right] \tag{10}$$

if $\overline{V}(\underline{x})$ is constant for all points equidistant from the design origin, then the design is slope rotatable over all direction (SROALD). For fair comparison of designs of different sizes, we scale the average slope variance. This is called the scaled average slope variance(SASV); see, Park [15].

Let $h(\underline{x})$denote the SASV, then

$$\begin{aligned} h(\underline{x}) &= \frac{N}{\sigma^2}\overline{V}(\underline{x}) \\ &= \frac{N}{k} tr\left[J(X'X)^{-1}J'\right] \end{aligned} \tag{11}$$

For design comparison, smaller values from (11) are preferred to larger values.

2B Central Composite Design (CCD)

A CCD comprises a factorial part, F consisting of $2^{k-q} (q \geq 0)$ units of at least resolution V (a situation where the main effects and two-factor interactions are not aliased with any other main effects or two-factor interactions) with each point replicated n_F times, which is usually called the cube. The levels of the factors are coded $(\pm 1, \pm 1)$, an axial part consisting of $2k$ units on the axis of each factor at a distance, α, from the centre of the design, $[(\pm\alpha, 0), (0, \pm\alpha)]$ usually called the star, with each point replicated n_α times and n_0 replication of the centre points, $(0, 0, \ldots, 0)$; all of which give a total of $N = n_F 2^{k-q} + n_\alpha 2k + n_0$; $\alpha-$ values are chosen based on some design criteria such as rotatability, slope-rotatability. The condition for a CCD to be slope rotatable over axial direction is as follows:

$$[2(F+n_0)]\,\alpha^8 - [4kF]\,\alpha^6 - F\,[N(4-k) + kF - 8(k-1)]\,\alpha^4 + \left[8(k-1)F^2\right]\alpha^2 - 2F^2(k-1)(N-F) = 0 \tag{12}$$

Rotatable $\subset$ slope rotatable over all directions. This implies that all rotatable designs are slope rotatable over all directions but the reverse is not true. The CCD which satisfy (12) are also slope rotatable over all directions; see Hader and Park [7], Park [15] and Ying, Pukelsheim and Draper [17].

2C Extended Central Composite Design (ECCD)

The ECCD is made up of a factorial part, F consisting of $2^{k-q}(q \geq 0)$ units of at least resolution V with each point replicated n_F times, an axial part consisting of $4k$ units on the axis of each factor from the centre of the design, with each point replicated n_α times and n_0 replication of the centre points, $(0,0,\ldots,0)$; which give a total of $M = n_F 2^{k-q} + n_\alpha 4k + n_0$. In ECCD two numbers represent the axial distance. Let the two numbers representing the axial distance be denoted by α_1 and α_2, such that $0 \leq \| \alpha_1 \| \leq \| \alpha_2 \| \leq r$. The condition for ECCD to be slope rotatable over axial direction is

$$2(F+2k+n_0)(\alpha_1^8+\alpha_2^8) - 8k(\alpha_1^6\alpha_2^2+\alpha_1^2\alpha_2^6) + 4(F+2k+n_0)\alpha_1^4\alpha_2^4 - 4kF(\alpha_1^6+\alpha_1^4\alpha_2^2+\alpha_1^2\alpha_2^4+\alpha_2^6) - F\{4F - 4k^2 + k(8-n_0) + 4(2+n_0)\}(\alpha_1^4+\alpha_2^4) + 16(k-1)F\alpha_1^2\alpha_2^2 + 8(k-1)F^2(\alpha_1^2+\alpha_2^2) - 2(k-1)F^2(4k+n_0) = 0 \quad (13)$$

The ECCD has slope rotatability over all direction, regardless of the values of α_1, α_2 and the number of centre points, n_0 see,Kim and Park [11].

3 Methodology

As mentioned earlier, the SASVQ plots shall be used to compare the designs. Because of its relevance in this work we shall briefly review it. A set of points are randomly generated on a sphere, $S(r)$ of radius r inside a region of interest,R, $S(r) = \{\underline{x} = \sum_{i=1}^{k} x_i^2 = r^2\}$, and then obtaining the value of $h(\underline{x}|r)$, that is the value of $h(\underline{x})$ at each of the randomly generated points. The random selection of points is achieved by using spherical coordinates. Any point $\underline{x} = (x_1, x_2, \ldots, x_k)$ on $S(r)$ can be represented using $k-1$ independent spherical coordinates $\theta_1, \theta_2, \ldots, \theta_{k-1}$ such that

$$\begin{aligned}
x_1 &= r\cos\theta_1, \\
x_2 &= r\ sin\ \theta_1,\ cos\ \theta_2, \\
x_3 &= r\sin\ \theta_1,\ sin\ \theta_2, \cos\ \theta_3, \\
&\vdots \\
x_{k-2} &= r\sin\ \theta_1,\ sin\ \theta_2, \ldots, \sin\ \theta_{k-3}\cos\ \theta_{k-2}, \\
x_{k-1} &= r\sin\ \theta_1,\ sin\ \theta_2, \ldots, \sin\ \theta_{k-3}\sin\ \theta_{k-2}\cos\ \theta_{k-1}, \\
x_k &= r\sin\ \theta_1,\ sin\ \theta_2, \ldots, \sin\ \theta_{k-3}\sin\ \theta_{k-2}\sin\ \theta_{k-1},
\end{aligned}$$

where $0 \leq \theta_1 \leq \theta_2 \leq \pi, \ldots, 0 \leq \theta_{k-2} \leq \pi, 0 \leq \theta_{k-1} \leq 2\pi$ (see, for example Edwards,[6]).
Values of $\theta_1, \theta_2, \ldots, \theta_{k-2}, \theta_{k-1}$ are randomly generated from independent uniform distribution such that $\theta_i \sim U(0,\pi), i = 1,2,\ldots,k-2;\ \theta_{k-1} \sim U(0,2\pi)$. For a chosen r, we obtain $x_1, x_2, \ldots, x_k$ which are used to evaluate $h(\underline{x}|r)$; see also, Borkowski [2]. Using this principle, a large number of points are chosen to obtain a sample, $H(r)$ consisting of values of $h(\underline{x})$ on $S(r)$. Then the quantiles of $H(r)$ are obtained. Plots of the quantiles of $H(r)$ versus $p, 0 \leq p \leq 1$ can be obtained for any value of r within the region R. The first quartile $(p = 0.25)$, the median $(p = 0.50)$, the third quartile $(p = 0.75)$ and so on can be obtained from the plots. Using this method, we obtain the distribution of the SASV inside the region R. Also, more than one design can be compared on the basis of their slope estimation capabilities by superimposing their respective quantiles of $H(r)$ inside R . This is called the combined quantile plots. We used MATLAB to generate uniform random numbers, obtain the values of SASV, the quantiles of $H(r)$ and the combined quantile plots. MATLAB is powerful and efficient in handling matrices and graphics.

4 Design Comparison

We compare the slope estimation capabilities of the two competing designs (CCD and ECCD) at multiple radii. The Design matrix of the CCD (D1) and ECCD (D2) for $k = 3$ and $n_0 = 1$ are shown below.

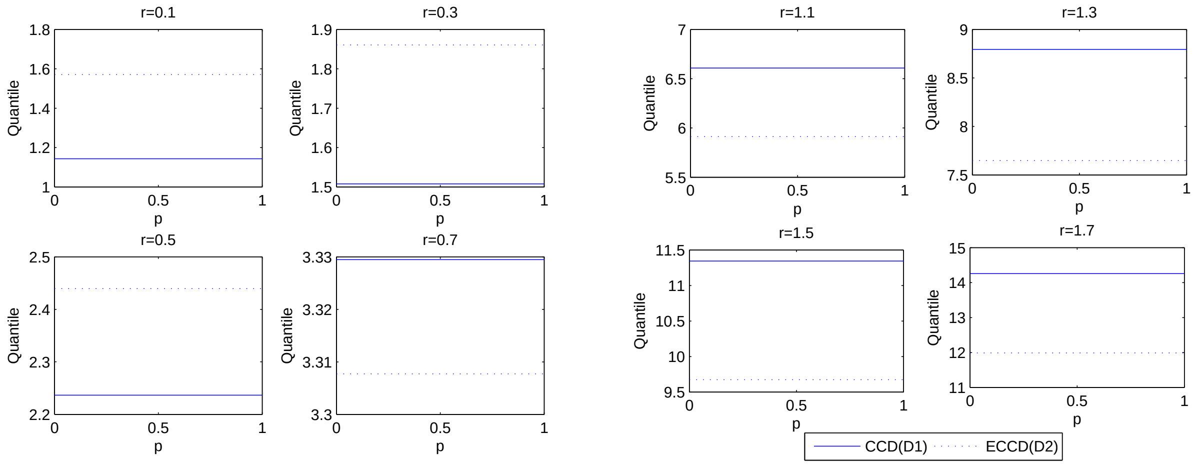

Fig. 1: Combined quantile plots for the slope rotatable CCD and ECCD

$$D1=\begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ -1.682 & 0 & 0 \\ 1.682 & 0 & 0 \\ 0 & -1.682 & 0 \\ 0 & 1.682 & 0 \\ 0 & 0 & -1.682 \\ 0 & 0 & 1.682 \\ 0 & 0 & 0 \end{bmatrix} D2=\begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ -0.1 & 0 & 0 \\ 0.1 & 0 & 0 \\ 0 & -0.1 & 0 \\ 0 & 0.1 & 0 \\ 0 & 0 & -0.1 \\ 0 & 0 & 0.1 \\ -1.682 & 0 & 0 \\ 1.682 & 0 & 0 \\ 0 & -1.682 & 0 \\ 0 & 1.682 & 0 \\ 0 & 0 & -1.682 \\ 0 & 0 & 1.682 \\ 0 & 0 & 0 \end{bmatrix}$$

The two designs are rotatable which implies SROAD. 10000 points are randomly selected on$S(r) = \{\underline{x} = \sum_{i=1}^{k} x_i^2 = r^2\}$, for each radius $r(= 0.1, 0.3, \ldots, 1.7)$. Plots of the quantiles of $H(r)$ are obtained. Fig. 1 shows the SASVQ plots. The plots correspond respectively to $r = 0.1, 0.3, \ldots, 1.7$. From the plots in Fig. 1, the average slope variance,$h(\underline{x})$ is stable (constant) for the two designs. This implies equal precision at all points $(x_1, x_2, \ldots, x_k)$ equidistant from the design origin (slope rotatability). Secondly, as r increases from 0.1 to 1.7, the quantiles of $h(\underline{x})$ also increase for all values of p. For $r \leq 0.5$, the SASVQ plots of the CCD are below that of the ECCD. The CCD have lower slope variance than the ECCD. Therefore, the former performs better than the later. But for $0.7 \leq r \leq 1.7$, the CCD are above the ECCD. The value of $h(\underline{x})$ for CCD is greater than that of ECCD. Hence, for these values of r , ECCD performs better than the CCD in terms of slope estimation.

5 Conclusion

The quantile plot is an effective graphical method for evaluating and comparing response surface designs when the assumptions in equations (1) and (2) hold. It can be used to prove constant slope variance. When interest is in slope estimation of the response surface at any specified direction, slope rotatability over all direction is a desirable criterion. Both CCD and ECCD have good statistical properties like rotatability and slope rotatability. We obtained slope rotatable CCD and ECCD over all direction and used the combined quantile plots to compare the designs on a sphere of radius $S(r) = \{\underline{x} = \sum_{i=1}^{k} x_i^2 = r^2\}$. In terms of the slope estimation capability, we found that the CCD is better than the ECCD near the design centre. However, the ECCD performs better than the CCD as one approaches the design perimeter.

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