2.1 INTRODUCTION

Hader and Park (1978) introduced 'Slope Rotatable Central Composite Designs' as an analogue of Box-Hunter second order central composite rotatable designs. They proved that the slope-rotatability can be achieved simply by adjusting the axial point distances (a) in central composite design, so that the variance of the estimate of pure quadratic coefficients is one-fourth the variance of the estimated mixed second order coefficients. They have constructed slope rotatable central composite designs (SRCCDs) for $2 \leq v \leq 8$ ($v$ stands for number of factors).

We generalise slope rotatable central composite design to second order slope rotatable design (SOSRD) on
lines similar to the general EHSORD. Then we derive the conditions for a design matrix to form a HPSOSRD. We try to evolve general methods of construction and analysis of SOSRD. We also try to obtain designs in parts with HP slope and BH response rotatability properties simultaneously.

2.2 SECOND ORDER SLOPE ROTATABLE DESIGN

In this section we generalise SRCCD to SOSRD and derive the conditions to be satisfied by SOSRD.

2.2.1 Conditions for Slope Rotatability in General Second Order Response Surface Design:

Let us consider a general second order response surface as

\[ Y(x) = b_0 + \sum_{i=1}^{v} b_i x_i + \sum_{i<j} b_{ij} x_i x_j + e \]  

(2.2.1)

where e's are independent random errors with same mean zero and variance \( \sigma^2 \).

Let us consider the following N design points in \( v \)-factors for fitting the above surface:
The object of the slope rotatability is to estimate the first order partial derivatives of \( Y(x) \) with respect to each of the independent variables with certain desirable criteria.

We define the slope rotatability criterion in general second order response surface design as follows:

Def. of SOSRD: A general second order response surface design is said to be a SOSRD if the variance of the estimate of first order partial derivative of \( Y(x) \) with respect to each of independent variables \( (x_i) \) is only a function of the distance \( (d^2 = \sum_{i=1}^{v} x_i^2) \) of the point \( (x_1, x_2, \ldots, x_v) \) from the origin (centre).
Let $y_1, y_2, \ldots, y_N$ be the $N$ observations obtained from the above $N$ design points in (2.2.2). To obtain the fit of the surface through the method of least squares, we have to solve the following normal equations (c.f. Das and Giri, 1986, p. 309).

$$\sum y = N b_0 + b_1 \sum x_1 + b_2 \sum x_2^2 + \ldots + b_{11} \sum x_1^2 +$$

$$b_{22} \sum x_2^2 + \ldots + b_{12} \sum x_1 x_2 + \ldots$$

$$\sum x_1 y = b_0 \sum x_1 + b_1 \sum x_1^2 + b_2 \sum x_1 x_2 + \ldots +$$

$$b_{11} \sum x_1^3 + b_{22} \sum x_1 x_2^2 + \ldots + b_{12} \sum x_1^2 x_2 + \ldots$$

$$\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$$

$$\sum x_1^2 y = b_0 \sum x_1^2 + b_1 \sum x_1^3 + b_2 \sum x_1^2 x_2 + \ldots + b_{11} \sum x_1^4 +$$

$$b_{22} \sum x_1^2 x_2^2 + \ldots + b_{12} \sum x_1^3 x_2 + \ldots$$

$$\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$$

$$\sum x_1 x_2 y = b_0 \sum x_1 x_2 + b_1 \sum x_1^2 x_2 + \ldots + b_{11} \sum x_1^3 x_2 + \ldots +$$

$$b_{12} \sum x_1^2 x_2^2 + b_{13} \sum x_1^2 x_2 x_3 + \ldots$$

$$\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \quad (2.2.3)$$

All the summations in the above expressions are over the design points.
Further we impose the following simple symmetry conditions on the design points (2.2.2) to simplify the solutions of the above normal equations as in the case of SORD (c.f. Das and Giri, 1986, p. 309).

A. \[ \sum x_i = 0, \quad \sum x_i x_j = 0, \quad \sum x_i^3 = 0, \]

\[ \sum x_i x_j x_k = 0, \quad \sum x_i^2 x_j x_k = 0, \quad \sum x_i^3 x_j = 0, \]

\[ \sum x_i x_j x_k x_L = 0 \text{ etc., for } i \neq j \neq k \neq L \]

B (i). \[ \sum x_i^2 = \text{constant} = N \lambda_2 \]

(ii). \[ \sum x_i^4 = \text{constant} = cN \lambda_4 \]

C. \[ \sum x_i^2 x_j^2 = \text{constant} = N \lambda_4 \quad \text{ ... (2.2.4)} \]

where \( c, \lambda_2 \) and \( \lambda_4 \) are constants. Using these symmetry conditions we can easily obtain the estimates of the parameters (c.f. Das and Giri, 1986, pp. 309-310) as

\[ \hat{b}_0 = \frac{\lambda_4(c+v-1)\sum y - \lambda_2 \sum (\sum x_i^2 y)}{N \left( \lambda_4(c+v-1) - v \lambda_2^2 \right)} \]

\[ \hat{b}_i = \frac{\sum x_i y}{N \lambda_2} \quad (i = 1, 2, \ldots, v) \]
\[ \hat{b}_{ij} = \frac{\sum x_i x_j y}{N \lambda_4} \quad (i \neq j = 1, 2, ..., v) \]

\[ \hat{b}_{11} = \frac{\sum x_i^2 y}{(c-1)N \lambda_4} - \frac{\lambda_2 \lambda_4 (c-1) \sum y - \sum (\sum x_i^2 y) \left( \lambda_2^2 - \lambda_4 \right)}{(c-1)N \lambda_4 \sqrt{\lambda_4 (c+v-1)} - v \lambda_2^2} \]

... (2.2.5)

We can obtain variances and covariances of the estimates (c.f. Das and Giri, 1986, p. 311) as

\[ \text{Var}(\hat{b}_0) = \frac{\lambda_4 (c+v-1) \sigma^2}{N \sqrt{\lambda_4 (c+v-1) - v \lambda_2^2}} \]

\[ \text{Var}(\hat{b}_1) = \frac{\sigma^2}{N \lambda_2} \]

\[ \text{Var}(\hat{b}_{1j}) = \frac{\sigma^2}{N \lambda_4} \]

\[ \text{Var}(\hat{b}_{11}) = \frac{\sigma^2}{(c-1)N \lambda_4} \times \left[ \frac{\lambda_4 (c+v-2) - (v-1) \lambda_2^2}{\lambda_4 (c+v-1) - v \lambda_2^2} \right] \]

\[ \text{Cov}(\hat{b}_0, \hat{b}_{11}) = -\frac{\lambda_2 \sigma^2}{N \sqrt{\lambda_4 (c+v-1) - v \lambda_2^2}} \]
\[
\text{Cov}(\hat{b}_{i1}, \hat{b}_{jj}) = \frac{(\lambda_2^2 - \lambda_4^4)\sigma^{-2}}{(c-1)N \lambda_4 \lambda_4 (c+v-1) - v \lambda_2^2}
\]

and other covariances vanish. \[\text{... (2.2.6)}\]

An inspection of the variance of \(\hat{b}_0\) shows that a necessary condition for the existence of a second order design is

\[
\lambda_4(c+v-1) - v \lambda_2^2 > 0
\]

which leads to the condition,

\[
\frac{\lambda_4^2}{\lambda_2^2} > \frac{v}{c+v-1} \quad \text{(non-singularity condition)}. \quad \text{... (2.2.7)}
\]

For second order model

\[
\frac{\partial \hat{Y}}{\partial x_1} = \hat{b}_1 + 2\hat{b}_{11}x_1 + \sum_{j \neq 1} \hat{b}_{1j} x_j \quad \text{... (2.2.8)}
\]

\[
\mathbb{V}\left(\frac{\partial \hat{Y}}{\partial x_1}\right) = \mathbb{V}(\hat{b}_1) + 4x_1^2\mathbb{V}(\hat{b}_{11}) + \sum_{j \neq 1} x_j^2\mathbb{V}(\hat{b}_{1j}) \quad \text{... (2.2.9)}
\]
The condition for R.H.S. of (2.2.9) to be a function of 
\[ d^2 = \sum_{1}^{v} x_i^2 \] alone (for Hader and Fark slope rotatability) 
is clearly,

\[ V(\hat{b}_{11}) = \frac{1}{4} V(\hat{b}_{1j}) \quad \ldots (2.2.10) \]

(2.2.4), (2.2.6) and (2.2.10) lead to the condition

\[ \lambda_4 \sum_{c}(5-c) - (c-3)^2 \sum \lambda_2 \sum_{(c-5)}+4 \sum = 0 \quad \ldots (2.2.11) \]

Therefore (2.2.4), (2.2.7) and (2.2.11) give a set of 
conditions for HP slope rotatability in any general 
second order response surface design.

We note that for BHSORD (2.2.4), (2.2.7) and \( c = 3 \) 
are the conditions to be satisfied by the design matrix 
(2.2.2). Now we have derived that for HPSOSRD (2.2.4), 
(2.2.7) and (2.2.11) are the conditions to be satisfied by 
the design matrix (2.2.2). Symmetry conditions (2.2.4) and 
non-singularity condition (2.2.7) are needed for both types 
of rotatabilities. We have to only replace third condition 
\( c = 3 \) in BH second order rotatability by the new condi-
tion (2.2.11) for obtaining HP second order slope rotata-
bility.

Note: We note that with \( c = 5 \) the Hader and Park condi-
tion (2.2.11) is independent of \( v \) and it reduces 
to \[ \lambda_4 = \lambda_2 \frac{2}{2} \].
2.2.2 **Classification of SOSRDs:**

Slope rotatability conditions (2.2.4), (2.2.7) and (2.2.11) depend upon the design parameters namely
(i) the coded levels of the factors $\sqrt{0}, \pm 1, \pm a$ etc. in (2.2.27),
(ii) the slope rotatability parameter ($c$), and
(iii) the number of central points ($n_o$). If we fix any one of the above three main parameters ($n_o$, $c$ or $a$) the remaining two parameters will automatically get fixed through (2.2.4), (2.2.7) and (2.2.11). For convenience of easy reference we classify SOSRD into three types called Type-I, Type-II and Type-III as follows.

(1) **Type-I SOSRD:**

If we first fix $n_o$ and then determine $a$ and $c$ accordingly for a second order response surface design to satisfy the conditions of SOSRD (2.2.4), (2.2.7) and (2.2.11), we refer to such SOSRD as Type-I SOSRD.

(1a) **Approximate Type-I SOSRD:**

In Type-I SOSRD, we are fixing $n_o$ and determining $a$ and $c$ suitably to achieve slope rotatability. But the level ($a$) as obtained in the design may have a large number of decimal places, for example the level of the factors may have to be taken as 4.25629572041 for exact Type-I SOSRD.
But maintaining this level exactly in practical situations may be difficult. In such cases we round off the level \(a\) to very few decimal places (above example level to (say) 4.3) and accordingly redetermine \(c\). Then we study sensitivity of the spherical variance function (2.2.9) for disturbances that occur due to the above minor modifications in the values of \(a\) and \(c\). The variance function (2.2.9) may now be of the form

\[
V \left( \frac{\partial Y}{\partial x_1} \right) = \varphi(d^2) + \epsilon
\]

where \(\epsilon\) is the disturbance term. If \(\epsilon\) is negligibly small, we may call the modified Type-I SOSRD as Approximate Type-I SOSRD.

2. **Type-II SOSRD:**

If we first fix conveniently \(c\) apriori within its admissible range (analogous to \(c=3\) in BHSORD) and then determine \(a\) and \(n_0\) (if \(n_0\) turns out to be a positive integer) suitably for a second order response surface design to satisfy the conditions of SOSRD (2.2.4), (2.2.7) and (2.2.11), we refer to such SOSRD as Type-II SOSRD.
(2a) Nearly Type II SOSRD:

For given \( v \) if \( n_0 \) is non-integral positive real number, we take \( \lfloor n_0 \rfloor \) or \( \lfloor n_0 \rfloor + 1 \) (\( \lfloor n_0 \rfloor \) - Gauss symbol denoting integral part of \( n_0 \)) central points and call such designs Nearly Type-II SOSRD. The extent of disturbance in the spherical variance function of such designs will be studied through sensitivity of the spherical variance function of the estimated slope to small changes in the value of \( n_0 \).

Note: We note that with \( c=5 \), the Hader and Park condition (2.2.11) is independent of \( v \) and it reduces to \( \lambda_4 = \lambda_2^2 \).

(3) Type-III SOSRD:

If we first fix conveniently \( a \) and determine \( n_0 \) (if \( n_0 \) turns out to be a positive integer) suitably for a second order response surface design to satisfy the conditions of SOSRD (2.2.4), (2.2.7) and (2.2.11), we refer to such SOSRD as Type-III SOSRD.

(3a) Nearly Type-III SOSRD:

For given \( v \) if \( n_0 \) is a non-integral positive real number, we take \( \lfloor n_0 \rfloor \) or \( \lfloor n_0 \rfloor + 1 \) central points and
call such designs Nearly Type-III SOSRD. The extent of disturbance in the spherical variance function of such designs will be studied through sensitivity of the variance function of the estimated slope to small changes in the value of $n_0$.

2.3 ANALYSIS OF SOSRD

Suppose the general second order response surface

$$Y(x) = b_0 + \sum_{i=1}^{v} b_i x_i + \sum_{i} \sum_{j} b_{ij} x_i x_j + e$$

is to be fitted with the design points (2.2.2) satisfying only the symmetry conditions (2.2.4). The normal equations to be solved for general second order response surface are given in (2.2.3). The estimates of parameters are given in (2.2.5). The variances and covariances of estimates of the parameters are given in (2.2.6). The relevant Analysis of variance table (A.V. Table) to test the validity of the second order model and to obtain an estimate of error variance is as follows (c.f. Das and Giri, 1986, p. 313).
### A.V. Table (2.1)

<table>
<thead>
<tr>
<th>Source</th>
<th>d.f.</th>
<th>S.S.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Due to regression Coefficients</td>
<td>$2v+v_c_2$</td>
<td>$b_0 \sum y + \sum b_i (\sum x_i y)$ + \sum b_j (\sum x_j y) - c.f.</td>
</tr>
<tr>
<td>Deviation from regression or lack of fit</td>
<td>$N'-2v-v_c_2-1$</td>
<td>Obtained by subtraction normally. ($N'$ = number of distinct treatment combinations).</td>
</tr>
<tr>
<td>Error</td>
<td>$N-N'$</td>
<td>Obtained independently adopting methods appropriate to the actual design.</td>
</tr>
<tr>
<td>Total</td>
<td>$N-1$</td>
<td>$\sum y^2 - c.f.$</td>
</tr>
</tbody>
</table>

For given SOSRD the concerned parameters $v$, $a$, $c$, $n_0$, $N$ are known. $\lambda_4$, $\lambda_2$ can be evaluated. The normal equations for SOSRD can be obtained from (2.2.3) using symmetry conditions (2.2.4) and slope rotatability condition (2.2.11). We can obtain the estimates of the parameters.
from (2.2.5) on further using (2.2.11). Variances and Covariances of estimates of the parameters in (2.2.5) are obtained from (2.2.6) on further using (2.2.11).

The Analysis of variance can be carried out as indicated above. The standard errors of the estimates can be estimated using the estimate of the error variance $\hat{\sigma}^2$ from Analysis of variance.

Further

\[ V\left( \frac{\partial \hat{Y}}{\partial x_1} \right) = V(\hat{b}_1) + \sum_1^x x_i^2 V(\hat{b}_{ij}). \]

\[ = \frac{1}{N}\left[ \frac{\lambda_4 + \lambda_2 \sigma^2}{\lambda_2 \lambda_4} \right]. \ldots (2.3.1) \]

\[ V\left( \frac{\partial \hat{Y}}{\partial x_1} \right) \]

can also be estimated using (2.3.1) and $\hat{\sigma}^2$ from the Analysis of variance.