CHAPTER - 4
RESPONSE SURFACE DESIGN MODEL REDUCTION USING SOBOL INDICES
CHAPTER- 4

4.1 INTRODUCTION

Sobol indices are the global sensitivity indices. These indices can be evaluated by decomposing variance based on the input-output relationship between the response and input variables. From the model, this index measures the contribution of individual components variance to the variance of the output variable. In general, Sobol’s method is computationally expensive and these indices do not provide a complete characterization of the sensitivity.

In this chapter an attempt is made to study the sobol indices and the proportion of the variances of estimated parameters and the response in case of first order and second order response surface design model are presented. These are illustrated with suitable examples.

4.2 DERIVATION OF SOBOL INDICES FOR FIRST ORDER RESPONSE SURFACE DESIGN MODEL:

Consider the following first order response surface design model in v factors

\[ Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_v X_v + \varepsilon \]  \hspace{1cm} (4.2.1)

It can be expressed as

\[ \underline{y} = X\beta + \varepsilon \]

Where,

\[ \underline{y} = (Y_1, Y_2 \ldots Y_N)' \] is the vector of observations,
\( X_u = (1, x_{u1}, x_{u2} \ldots x_{uv}) \) is the \( u \)th row of \( X \)

\( \beta = (\beta_0, \beta_1, \beta_2 \ldots \beta_v) \) is the vector of parameters, and

\( \varepsilon = (\varepsilon_1, \varepsilon_2 \ldots \varepsilon_N)' \) is the vector of random errors.

Assume \( E(\varepsilon) = 0, D(\varepsilon) = \sigma^2 I \) and \( \varepsilon \sim N(0, \sigma^2) \).

The least square estimate of \( \beta \) is given by

\[
\hat{\beta} = (X'X)^{-1}X'Y \tag{4.2.2}
\]

The estimated response at \( u \)th design point is

\[
\hat{Y}_u = \hat{\beta}_0 + \hat{\beta}_1 x_{u1} + \hat{\beta}_2 x_{u2} + \ldots + \hat{\beta}_v x_{uv} \tag{4.2.3}
\]

and Variance-Covariance matrix of \( \hat{\beta} \) is given by

\[
V(\hat{\beta}) = (X'X)^{-1}\sigma^2 \tag{4.2.4}
\]

Where, the moment matrix of \( X \) is

\[
X'X = \begin{bmatrix}
N & \sum_{u=1}^{N} x_{u1} & \cdots & \sum_{u=1}^{N} x_{uv} \\
\vdots & \vdots & \ddots & \vdots \\
\sum_{u=1}^{N} x_{u1} & \sum_{u=1}^{N} x_{u1}^2 & \cdots & \sum_{u=1}^{N} x_{u1} x_{uv} \\
\vdots & \vdots & \ddots & \vdots \\
\sum_{u=1}^{N} x_{uv} & \sum_{u=1}^{N} x_{u1} x_{uv} & \cdots & \sum_{u=1}^{N} x_{uv}^2
\end{bmatrix} \tag{4.2.5}
\]

The variance of the predicted response at the \( u \)th point is

\[
V(\hat{Y}_u) = V(\hat{\beta}_0) + \sum_{i=1}^{v} x_{ui}^2 V(\hat{\beta}_i) + \sum_{i=1}^{v} \sum_{j=1}^{v} x_{ui} x_{uj} \text{Cov}(\hat{\beta}_i, \hat{\beta}_j) \tag{4.2.6}
\]

\[
= \frac{\sigma^2}{N} + X'(X'X)^{-1}X\sigma^2
\]
A reasonable criterion for the choice of a first order design is the minimization of the variance of $\hat{Y}_u$. More specifically, we seek for a design for which $X'(X'X)^{-1}X$ is as small as possible with in the region $R$, where the first order model adequately represent the true response.

The variance of the estimated response $V(\hat{Y}_u)$ is decomposed into partial variances associated with each of the input variables $X_1, X_2, \ldots, X_v$ and its associated parameters of the model as

$$V(\hat{Y}_u) = V(\hat{\beta}_0) + \sum_{i=1}^{v} \xi_i^2 V(\hat{\beta}_i) + \sum_{i=1}^{v} \sum_{j=1}^{v} \xi_i \xi_j Cov(\hat{\beta}_i, \hat{\beta}_j) \quad (4.2.7)$$

Let, the variance of the estimated response $V(\hat{Y}_u) = \sigma^2$. Then the sobol indices $S_i$'s corresponding to each of the component are evaluated, which are given as

$$S_0 = V(\hat{\beta}_0) / V(\hat{Y}_u);$$

$$S_i = \left[ \sum_{i=1}^{v} \xi_i V(\hat{\beta}_i) \right] / V(\hat{Y}_u); \quad (4.2.8)$$

$$S_{ij} = \left[ \sum_{i=1}^{v} \sum_{j=1}^{v} \xi_i \xi_j Cov(\hat{\beta}_i, \hat{\beta}_j) \right] / V(\hat{Y}_u)$$

The $\sum_{i=1}^{v} \xi_i$, $\sum_{i=1}^{v} \sum_{j=1}^{v} \xi_i \xi_j$ and the variances of the parameters are not in compressed form to evaluate theoretically, if there are no restrictions on moment matrix of first order response surface design. Even though it is not in simplified form but, it is possible to reduce the size of the model by eliminating the insignificant component from the model.

Towards reaching to orthogonality and obtaining the simplified formulae for the sobol indices, the following conditions are imposed on the moment matrix
\[ \sum_{u=1}^{N} x_{ui} = 0; \quad \sum_{u=1}^{N} x_{ui} x_{uj} = 0; \quad i \neq j = 1,2 \ldots v \quad \text{let} \quad \sum_{u=1}^{N} x_{ui}^2 = N\lambda_2 \quad (4.2.7) \]

Then, the variance – covariance matrix \( X'X \) can be obtained as

\[
X'X = \begin{bmatrix}
N & 0 \\
0 & N\lambda_2 I
\end{bmatrix}
\quad (4.2.8)
\]

The variance of the estimated response at the \( u \)th design point is

\[ V(\hat{Y}_u) = V(\hat{\beta}_0) + \sum_{i=1}^{v} x_{ui}^2 V(\hat{\beta}_i) \quad (4.2.9) \]

Where, \( V(\hat{\beta}_0) = \sigma^2 / N; \quad V(\hat{\beta}_i) = \sigma^2 / N\lambda_2 \) for \( i = 1,2, \ldots v \).

Then, the sobol indices corresponding to each of the component are

\[ S_0 = N^{-1} \quad \text{and} \quad S_i = \frac{x_{ui}^2}{N\lambda_2 \sigma^2} \quad \text{for} \ i = 1,2, \ldots v \]

The Sobol indices \( S_0 \) and \( S_i \) satisfy the condition \( S_0 + \sum_{i=1}^{v} S_i = 1 \). Even though the sobol indices obtained are in a simplified form in the above case but its evaluation is difficult due to the part of the components which contains \( x_{ui} \)'s. Elimination of insignificant component from the model in case of orthogonal design is difficult due to their proportion of variance indices are same.

The proportion of variance indices are used to obtain the sobol indices in case of non-orthogonal design and orthogonal design are illustrated through the examples 4.2.1 and 4.2.2, respectively.

**EXAMPLE 4.2.1:** Consider the data of responses at different design points of first order response surface model with four factors as
<table>
<thead>
<tr>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_3$</th>
<th>$X_4$</th>
<th>$Y$</th>
</tr>
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<td>120</td>
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<tr>
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<td>-1</td>
<td>-1</td>
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<tr>
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<td>-1</td>
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</tr>
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<td>-1</td>
<td>-1</td>
<td>140</td>
</tr>
<tr>
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<td>-1</td>
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<td>1</td>
<td>141</td>
</tr>
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<td>-1</td>
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<tr>
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<td>1</td>
<td>-1</td>
<td>1</td>
<td>402</td>
</tr>
</tbody>
</table>

The estimates of the un-standardized parameters are $\hat{\beta}_0 = 328.3$; $\hat{\beta}_1 = -7.365$; $\hat{\beta}_2 = 2.97$; $\hat{\beta}_3 = 2.57$; and $\hat{\beta}_4 = -51.07$. The variance of the estimated response is 11202.61. The proportion of variance indices ($s_i$'s) corresponding to estimated parameters and response are $s_0 = 0.0794$; $s_1 = 0.0662$; $s_2 = 0.06092$; $s_3 = 0.0878$; $s_4 = 0.0711$. It can be observed that the proportion of variance indices ($s_i$'s) are differing for the nonorthogonal design.
**EXAMPLE 4.2.2:** The effects of extraction time \( t \), solvent volume \( V \), ethanol concentration \( C \), and temperature \( T \) on the yield of deoiled rapeseed lecithin when fractionated with ethanol was studied a single-replicate 24 experiments was conducted augmented by three centre points. *Coded Variables are:* \( A = \frac{t - 10}{5} \); \( B = \frac{V - 7.5}{2.5} \); \( C = \frac{C_{on} - 95}{3} \); \( D = \frac{T - 20}{5} \).
<table>
<thead>
<tr>
<th>Natural Variables</th>
<th>Coded Variables</th>
<th>Responses</th>
</tr>
</thead>
<tbody>
<tr>
<td>t</td>
<td>V</td>
<td>C</td>
</tr>
<tr>
<td>15</td>
<td>10</td>
<td>98</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
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<td>5</td>
<td>92</td>
</tr>
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<td>92</td>
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<tr>
<td>5</td>
<td>10</td>
<td>92</td>
</tr>
</tbody>
</table>

The parameter estimates in the first order response surface model are obtained from the formula \( \hat{\beta} = (X'X)^{-1}X'Y \). The estimates of the un-standardized parameters are \( \hat{\beta}_0 = 17.9, \hat{\beta}_1 = 64, \hat{\beta}_2 = 2.55, \hat{\beta}_3 = 2.2; \) and \( \hat{\beta}_4 = 1.275 \).

The fitted first-order response surface model for Yield is

\[
\hat{Y}_u = \hat{\beta}_0 + \hat{\beta}_1 x_{u1} + \hat{\beta}_2 x_{u2} + \ldots + \hat{\beta}_v x_{uv}.
\]
The variance of the response is 17.30. The proportion of variance indices \(s_i\)'s corresponding to estimated parameters and response are \(s_0 = 1.08125; s_1 = 1.08125; s_2 = 1.08125; s_3 = 1.08125; s_4 = 1.08125\). It can be observed that, the proportion of variance indices \(s_i\)'s are same for the above orthogonal design.

4.3 DERIVATION OF PROPORTION OF VARIANCE INDICES FOR SECOND ORDER RESPONSE SURFACE MODEL:

Consider the following second-order response surface design model in \(v\) factors

\[
Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_v X_v + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \ldots + \beta_{vv} X_v^2 \\
+ \beta_{12} X_1 X_2 + \ldots + \beta_{v-1v} X_{v-1} X_v + \varepsilon
\]

(4.3.1)

It can be expressed as

\[
Y = X\hat{\beta} + \varepsilon
\]

(4.3.2)

Where,

\[
Y = (Y_1, Y_2 \ldots Y_N)' \text{ is the vector of observations,}
\]

\[
X_u = (1, x_{u1}, x_{u2} \ldots x_{uv}, x_{u1}^2, x_{u2}^2 \ldots x_{uv}^2, x_{u1}x_{u2} \ldots x_{uv-1}x_{uv}) \text{ is the } u^{th} \text{ row of } X
\]

\[
\beta = (\beta_0, \beta_1, \beta_2 \ldots \beta_v, \beta_{11}, \beta_{22} \ldots \beta_{vv}, \beta_{12} \ldots \beta_{v-1v})' \text{ is the vector of parameters}
\]

\[
\varepsilon = (\varepsilon_1, \varepsilon_2 \ldots \varepsilon_N)' \text{ is the vector of random errors.}
\]

Assume \(E(\varepsilon) = 0, D(\varepsilon) = \sigma^2 I\) and \(\varepsilon \sim N(0, \sigma^2)\).

The least square estimate of \(\beta\) is given by

\[
\hat{\beta} = (X'X)^{-1}X'Y
\]

(4.3.3)

The estimated response at the \(u^{th}\) design point is
\[
\hat{y}_u = \hat{\beta}_0 + \sum_{i=1}^{v} \hat{\beta}_i x_{ui} + \sum_{i=1}^{v} \hat{\beta}_{ii} x_{ui}^2 + \sum_{i,j=1}^{v} \hat{\beta}_{ij} x_{ui} x_{uj}
\] (4.3.4)

and Variance-Covariance matrix of \(\hat{\beta}\) is given by

\[
V(\hat{\beta}) = (X^\prime X)^{-1} \sigma^2
\] (4.3.5)

Where, the moment matrix of \(X\) is

\[
X^\prime X = \begin{bmatrix}
\end{bmatrix}
\] (4.3.6)

Where \([i]\), \([ij]\), \([ijk]\), \([ijkl]\), \([iijk]\) are terms related to sum of \(x_{ui}, x_{ui}x_{uj}, x_{ui}x_{uj}x_{uk}\), \(x_{ui}x_{uj}x_{uk}x_{ul}\), \(x_{ui}x_{ui}x_{ui}x_{uj}\) over the \(N\) design points.

Let \(S_0, S_i, S_{ii}\) and \(S_{ij}\) be the sobol indices corresponding to each of the components in the model (4.3.1) satisfying \(S_0 + \sum_{i=1}^{v} S_i + \sum_{i=1}^{v} S_{ii} + \sum_{i,j=1}^{v} S_{ij} = 1\). The evaluation of the sobol indices corresponding to each of the component is not in a compressed form for any second order response surface design. It is possible to evaluate the proportion of variances of estimated parameters and response for ranking the parameters in the model for any practical problem. The sobol indices can be evaluated by specifying design point \(x_{ui}\)'s to know the contribution of each component in the model. The size of the model can be reduced by eliminating the insignificant component from the model.

Towards reaching to near orthogonality, the following conditions are imposed on the moment matrix
\[ \sum_{u=1}^{N} x_{ui} = 0 \quad \sum_{u=1}^{N} x_{ui} x_{uj} = 0 \quad \sum_{u=1}^{N} x_{ui} x_{uj} = 0 \quad \sum_{u=1}^{N} x_{ui}^3 = 0 \]

\[ \sum_{u=1}^{N} x_{ui}^2 = 0 \quad \sum_{u=1}^{N} x_{ui} x_{uj}^2 = 0 \quad \sum_{u=1}^{N} x_{ui} x_{uj} x_{uk} x_{ul} = 0 \quad \text{if } i \neq j \neq k \neq l = 1, \ldots, v; \quad (4.3.7) \]

and let \( \sum_{u=1}^{N} x_{ui}^2 = N \lambda_2 \), \( \sum_{u=1}^{N} x_{ui}^4 = C N \lambda_4 \), \( \sum_{u=1}^{N} x_{ui}^2 x_{uj}^2 = N \lambda_4 \)

The variance – covariance matrix \( X'X \) is obtained

\[
X'X = \begin{bmatrix}
1 & 0 & \lambda_2 J & 0 \\
0 & \lambda_2 J & 0 & 0 \\
\lambda_2 J & 0 & [(c-1)I + J]\lambda_4 & 0 \\
0 & 0 & 0 & \lambda_4 I
\end{bmatrix} \quad (4.3.8)
\]

With

\[
(X'X)^{-1} = \begin{bmatrix}
\lambda_4 (c+v+1)\Delta^{-1} & 0 & (c+v-1)(c-1)\Delta^{-1} & 0 \\
0 & \lambda_2^{-1} I & 0 & 0 \\
-2\lambda_2 J\Delta^{-1} & 0 & Z_{xv} & 0 \\
0 & 0 & 0 & \lambda_2^{-1}
\end{bmatrix} \quad (4.3.9)
\]

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

and \( Z_{xv} = \frac{[(c+v-1)I - J]_{v,v}}{\lambda_4 (c-1)(c+v-1)} + \frac{[\lambda_2^2 (c+v-1)(c-1)I]}{[\lambda_4 (c+v-1) - k\lambda_2^2]} J_{k,k} \)

The variance of the estimated response is

\[
V(\hat{\bar{Y}}_u) = V(\hat{\beta}_0) + \sum_{i=1}^{v} x_{ui}^2 V(\hat{\beta}_i) + \sum_{i=1}^{v} x_{ui}^4 V(\hat{\beta}_{ii}) + \sum_{i<j}^{v} x_{ui}^2 x_{uj} V(\hat{\beta}_{ij})
\]

\[ + 2 \text{Cov}(\hat{\beta}_0, \hat{\beta}_{ii}) \sum_{i=1}^{v} x_{ui}^2 + 2 \text{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{ij}) \sum_{i<j}^{v} x_{ui}^2 x_{uj}^2 \quad (4.3.10) \]

Where,
\[ V(\hat{\beta}_0) = \left[ \lambda_4 (c+k-1)/N\Delta \right] \sigma^2 \]

\[ V(\hat{\beta}_i) = (1/N\lambda_2) \sigma^2 \]

\[ V(\hat{\beta}_{ij}) = (1/N\lambda_4) \sigma^2 \]

\[ \text{Cov}(\hat{\beta}_0, \hat{\beta}_{ij}) = [-\lambda_2 / N\Delta] \sigma^2 \]

\[ V(\hat{\beta}_{ii}) = \left[ \{\lambda_4(c+k-2)-(k-1)\lambda_2^2\} / \{N\lambda_4(c-1)\Delta\} \right] \sigma^2 \]

\[ \text{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{jj}) = \left[ (\lambda_2^2 - \lambda_4) / \{(c-1)N\lambda_4\Delta\} \right] \sigma^2 \]

Other covariance terms vanish.

\[
\text{if } \sum_{i=1}^{v} x_{ui}^2 = \rho^2 ; \text{ then } \sum_{i=1}^{v} x_{ui}^4 = \rho^4 - 2 \sum_{i<j} x_{ui}^2 x_{uj}^2
\]

Then, the variance of the estimated response is

\[
V(\hat{Y}_u) = V(\hat{\beta}_0) + \rho^2 V(\hat{\beta}_i) + (\rho^4 - 2 \sum_{i<j} x_{ui}^2 x_{uj}^2) V(\hat{\beta}_{ii}) + 2 \text{Cov}(\hat{\beta}_0, \hat{\beta}_{ii}) \rho^2 + 2 \text{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{jj}) \sum_{i<j} x_{ui}^2 x_{uj}^2
\]

\[
\Rightarrow V(\hat{Y}_u) = V(\hat{\beta}_0) + [V(\hat{\beta}_i) + 2\text{Cov}(\hat{\beta}_0, \hat{\beta}_{ii})] \rho^2 + V(\hat{\beta}_{ii}) \rho^4 + [V(\hat{\beta}_{ii}) - 2 V(\hat{\beta}_{ii}) + 2\text{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{jj})] \sum_{i<j} x_{ui}^2 x_{uj}^2
\]

The resulting variance of estimated response from the above equations is

\[
V(\hat{Y}_u) = \frac{\sigma^2}{N\Delta} \left[ \left( \frac{\Delta - 2\lambda_2^2}{\lambda_2^2} \right) \rho^2 + \left( \frac{\Delta - \lambda_2^2}{\lambda_4(c-1)} \right) \rho^4 - \{\Delta + \nu\lambda_2^2\} \right] + \left[ \frac{(c-3)}{(c-1)N\lambda_4} \sigma^2 \right] \sum_{i>j} x_i^2 x_j^2
\]
The proportion of variance indices (s_i's) corresponding to each of the parameter in the model are evaluated and the resulting values are

\[ s_0 = \frac{\lambda_4 (c + k - 1) / \Delta}{\Delta \left[ \frac{\Delta - \lambda_2^2}{\lambda_4 (c - 1)} - \frac{\Delta - 2 \lambda_2^2}{\lambda_2} \rho^2 + (\Delta + k \lambda_2^2) + \frac{(c - 3) \Delta}{(c - 1) \lambda_4} \sum_{i=1}^{k} x_i^2 x_j^2 \right]} \]

\[ s_i = \frac{1}{\lambda_2} \]

\[ s_{ij} = \frac{1}{\lambda_4} \]

\[ s_{ii} = \frac{\lambda_4 (c + k - 2) - (k - 1) \lambda_2^2}{\lambda_4 (c - 1) \left[ \frac{\Delta - \lambda_2^2}{\lambda_4 (c + k - 1) - k \lambda_2^2} \right]} \]

\[ \Delta \left[ \frac{\Delta - \lambda_2^2}{\lambda_4 (c - 1)} - \frac{\Delta - 2 \lambda_2^2}{\lambda_2} \rho^2 + (\Delta + k \lambda_2^2) + \frac{(c - 3) \Delta}{(c - 1) \lambda_4} \sum_{i=1}^{k} x_i^2 x_j^2 \right] \]

\[ s_{0} : s_{1} : s_{ii} = s_{ij} = \frac{\lambda_4 (c + v - 1)}{\Delta} : \frac{1}{\lambda_2} : \frac{1}{\lambda_4} : \frac{\lambda_4 (c + v - 2) - (v - 1) \lambda_2^2}{\lambda_4 (c - 1) \Delta} \]

(4.4.1)
\[ s_0 : s_j : s_{ii} : s_{ij} = \frac{\lambda_4 (c + v - 1)}{[\lambda_4 (c + v - 1) - v\lambda_2^2]} : \frac{1}{\lambda_2} : \frac{\lambda_4 (c + v - 2) - (v - 1)\lambda_2^2}{\lambda_4 (c - 1) [\lambda_4 (c + v - 1) - v\lambda_2^2]} \]

**Case-1**: Comparison of index \( s_i \) with index \( s_{ii} \)

From the ratio of (4.4.1), when \( s_i \) and \( s_{ii} \) are compared,

\[
s_i : s_{ii} = \frac{1}{\lambda_2} : \frac{1}{\lambda_4} \]

Where \( cN\lambda_4 = \sum x^4_m \) and \( N\lambda_2 = \sum x^2_m \)

\[ \Rightarrow \]

\[
s_i : s_{ij} = \frac{1}{\sum_{u=1}^{N} x^2_m} : \frac{c}{\sum_{u=1}^{N} x^4_m} \]

**Note:**

1. In general, for any design matrix, the condition \( \sum x^4_m \geq \sum x^2_m \) is satisfied

2. If \( \frac{1}{c} \sum_{u=1}^{N} x^4_m \geq \sum_{u=1}^{N} x^2_m \) then, \( s_i \geq s_{ii} \).

3. If \( \frac{1}{c} \sum_{u=1}^{N} x^4_m = \sum_{u=1}^{N} x^2_m \) then, \( s_i \geq s_{ii} \) and \( \sum_{i=1}^{v} s_i = \sum_{i=1}^{v} s_{ii} \)

**Case-2**: Comparison of index \( s_i \) with interaction index \( s_{ij} \)

From the ratio of (4.4.1), when \( s_i \) and \( s_{ij} \) are compared,

\[
s_i : s_{ij} = \frac{1}{\lambda_2} : \frac{[\lambda_4 (c + v - 2) - (v - 1)\lambda_2^2]}{\lambda_4 (c - 1) [\lambda_4 (c + v - 1) - v\lambda_2^2]} \]

\[
= \frac{1}{\lambda_2} : \frac{1}{\lambda_4} \times \frac{1}{(c - 1)} \times \frac{[\lambda_4 (c + v - 1) - v\lambda_2^2] - (\lambda_4 - \lambda_2^2)}{[\lambda_4 (c + v - 1) - v\lambda_2^2]} \]

\[
= \frac{1}{\lambda_2} : \frac{1}{\lambda_4} \times \frac{1}{(c - 1)} \times [1 - \frac{(\lambda_4 - \lambda_2^2)}{[\lambda_4 (c + v - 1) - v\lambda_2^2]}] \]
\[
\frac{1}{\lambda_2} : \frac{1}{\lambda_4} \times \frac{1}{(e - 1)} \times (1 - \delta)
\]
where \(\delta = \frac{(\lambda_4 - \lambda_2^2)}{[\lambda_4 (c + v - 1) - v\lambda_2^2]}\)

It can be noted from the above ratio that, for all \(c > 1\) and \(\delta\) is very small.

**Case-3**: Comparison of index \(s_{ii}\) with index \(s_{ij}\)

From the ratio of (4.4.1), when \(s_{ii}\) and \(s_{ij}\) are compared

\[
s_{ii} : s_{ij} = \frac{\lambda_4 (c + v - 2) - (v - 1)\lambda_2^2}{\lambda_4 ([c - 1] \cdot \Delta)} : \frac{1}{\lambda_4}
\]

\[
= \frac{[\lambda_4 (c + v - 2) - (v - 1)\lambda_2^2]}{(c - 1)[\lambda_4 (c + v - 1) - v\lambda_2^2]} : 1
\]

\[
= \frac{1}{(c - 1)} \times \frac{[\lambda_4 (c + v - 2) - (v - 1)\lambda_2^2]}{[\lambda_4 (c + v - 1) - v\lambda_2^2]} : 1
\]

\[
= \frac{1}{(c - 1)} \times (1 - \delta) \quad \text{where} \quad \delta = \frac{(\lambda_4 - \lambda_2^2)}{[\lambda_4 (c + v - 1) - v\lambda_2^2]}
\]

It can be noted that, when \(c > 1\), \(s_{ii} < s_{ij}\)

**Case-4**: Comparison of index \(s_0\) and index \(s_i\)

From the ratio of (4.4.1), when \(s_0\) and \(s_i\) are compared

\[
s_0 : s_i = \frac{\lambda_4 (c + v - 1)}{\Delta} : \frac{1}{\lambda_2}
\]

\[
\Rightarrow s_0 : s_i = \frac{\lambda_4 (c + v - 1)}{\lambda_4 (c + v - 1) - v\lambda_2^2} : \frac{1}{\lambda_2}
\]
\[ s_0 : s_i = \frac{1}{1 - \frac{v \lambda_2^2}{(c + v - 1) \lambda_4}} : \frac{1}{\lambda_2} \]

**Note:**

1. The comparison exists for non-standardized model and valid only if the conditions given in (4.3.6) are satisfied.
2. \[ \Delta = [\lambda_4 (c + v - 1) \lambda_4] > 0 \Rightarrow \lambda_4 (c + v - 1) > v \lambda_2^2 \]
3. If \( \lambda_2^2 \leq \lambda_4 \) and \( c \geq 1 \) then, \( s_0 < s_i \) for all \( \lambda_2 \geq 1 \).
4. If \( \lambda_2^2 \leq \lambda_4 \) and \( c = 1 \) then, \( s_0 > s_i \) for all \( \lambda_2 \geq 1 \).
5. If \( \lambda_2^2 = \lambda_4 \) and \( c = 1 \) then, \( s_0 \) is highly significant for all \( \lambda_2 \geq 1 \).

**Case-4:** Comparison of index \( s_0 \) and index \( s_{ii} \)

From the ratio of (4.4.1), when \( s_0 \) and \( s_{ii} \) are compared

\[ s_0 : s_{ii} = \frac{\lambda_4 (c + v - 1) \lambda_4 (c + v - 2) - (v - 1) \lambda_2^2}{\Delta} : \frac{\lambda_4 (c + v - 1) \lambda_4 (c + v - 2) - (v - 1) \lambda_2^2}{\Delta \lambda_4 (c - 1)} \]

\[ \Rightarrow s_0 : s_{ii} = \lambda_4 (c + v - 1) : \frac{c + v - 2}{c - 1} - \frac{v - 1}{c - 1} \lambda_2^2 \lambda_4 \]

\[ \Rightarrow s_0 : s_{ii} = \lambda_4 (c + v - 1) > \frac{c + v - 2}{c - 1} - \frac{v - 1}{c - 1} \lambda_2^2 \lambda_4 \quad \forall \lambda_4 > 1, \]

\[ \therefore s_0 > s_{ij} \quad \forall \lambda_4 > 1. \]

**Case-5:** Comparison of index \( s_0 \) and index \( s_{ij} \)

From the ratio of (4.4.1), when \( s_0 \) and \( s_{ij} \) are compared
s_0 : s_{ij} = \frac{\lambda_4 (c + v - 1)}{\Delta} : \frac{1}{\lambda_4}

= \frac{\lambda_4 (c + v - 1)}{\lambda_4 (c + v - 1) - v \lambda_2^2} : \frac{1}{\lambda_4}

It can be noted that \frac{\lambda_4 (c + v - 1)}{\lambda_4 (c + v - 1) - v \lambda_2^2} > 1 \text{ for } \forall \lambda_4 > 1 \text{ and}

\text{If } \frac{1}{\lambda_4} < 1 \text{ for } \forall \lambda_4 > 1 \therefore s_0 > s_{ij} \forall \lambda_4 > 1.

The computation of proportion of variance indices of estimated parameters to the response to obtain the sobol indices for second order Response surface designs in case of general, with restrictions but not rotatable and rotatable designs are illustrated through examples 4.3.1, 4.3.2, and 4.3.3 respectively.

**EXAMPLE 4.3.1:** Consider the following data of responses corresponding a second order response surface design with three factors is given below
<table>
<thead>
<tr>
<th>X_1</th>
<th>X_2</th>
<th>X_3</th>
<th>Y</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>2.83</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>-1</td>
<td>3.25</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>3.56</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>2.53</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>3.01</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>3.19</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>2.23</td>
</tr>
<tr>
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<td>0</td>
<td>1</td>
<td>2.65</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>3.06</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>2.57</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>-1</td>
<td>3.08</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>3.50</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>2.42</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>2.79</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
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<td>3.03</td>
</tr>
<tr>
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<td>-1</td>
<td>1</td>
<td>2.07</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>2.85</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>3.12</td>
</tr>
</tbody>
</table>

The estimates of the un-standardized parameters are $\hat{\beta}_0 = 51.74$, $\hat{\beta}_1 = 0.44$, $\hat{\beta}_2 = -0.209$, $\hat{\beta}_3 = -0.038$; $\hat{\beta}_{11} = 0.023$, $\hat{\beta}_{22} = 0.539$, $\hat{\beta}_{33} = 0.840$, $\hat{\beta}_{12} = 0.170$, $\hat{\beta}_{13} = -0.066$ and $\hat{\beta}_{23} = -0.513$. The variance of the estimated response is 0.165. The proportion of variance indices corresponding to the parameters are $s_0 = 0.3572$; $s_1 = 0.0198$; $s_2 = 0.0292$; $s_3 = 0.0235$; $s_{11} = 0.0547$, $s_{22} = 0.1559$, $s_{33} = 0.2715$, $s_{12} = 0.0405$. 

$s_{13} = 0.031$ and $s_{23} = 0.1134$ which are used for ranking the parameters $\beta_i$’s to reduce the model.

**EXAMPLE 4.3.2:** Consider the following data of responses corresponding to a second order response surface design with four factors
<table>
<thead>
<tr>
<th></th>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_3$</th>
<th>$X_4$</th>
<th>Y</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>63.03</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>62.19</td>
</tr>
<tr>
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<td>0</td>
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<td>0</td>
<td>0</td>
<td>64.01</td>
</tr>
<tr>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>61.60</td>
</tr>
<tr>
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<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>58.95</td>
</tr>
<tr>
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<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>78.34</td>
</tr>
<tr>
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<td>-1</td>
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<td>-1</td>
<td>-1</td>
<td>45.75</td>
</tr>
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<td>1</td>
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<td>-1</td>
<td>-1</td>
<td>72.66</td>
</tr>
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<td>-1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>46.36</td>
</tr>
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<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>68.62</td>
</tr>
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<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>35.16</td>
</tr>
<tr>
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<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>71.62</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>84.01</td>
</tr>
<tr>
<td>1</td>
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<td>1</td>
<td>-1</td>
<td>1</td>
<td>61.18</td>
</tr>
<tr>
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<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>77.78</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>61.15</td>
</tr>
<tr>
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<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
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</tr>
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<td>-1</td>
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<td>1</td>
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</tr>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>65.72</td>
</tr>
</tbody>
</table>

The estimates of the un-standardized parameters are $\hat{\beta}_0 = 62.70$, $\hat{\beta}_1 = 9.28$, $\hat{\beta}_2 = -4.62$, $\hat{\beta}_3 = -5.42$, $\hat{\beta}_4 = 5.22$, $\hat{\beta}_{22} = -94.13$, $\hat{\beta}_{33} = -94.13$, $\hat{\beta}_{44} = 27.6$. 
\( \hat{\beta}_{12} = 0.821, \hat{\beta}_{13} = -0.12, \hat{\beta}_{14} = -2.294, \hat{\beta}_{11} = 161.22, \hat{\beta}_{23} = -0.17, \hat{\beta}_{24} = 0.311, \) and \( \hat{\beta}_{34} = 0.367. \) The variance of the estimated response is 144.33. The proportion of variance indices corresponding to the parameters are \( s_0 = 118.35; s_1 = s_2 = s_3 = s_4 = 9.06; s_{11} = s_{22} = s_{33} = 2.8433; s_{12} = s_{13} = s_{14} = s_{23} = s_{24} = s_{34} = 9.02 \) which are used for ranking the parameters \( \beta_i \)'s to reduce the model.

**EXAMPLE 4.3.3:** Consider the following data with responses of a second order rotatable design with four factors as
<table>
<thead>
<tr>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_3$</th>
<th>$X_4$</th>
<th>Response</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>0</td>
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<tr>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>0</td>
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<td>1</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td>-1</td>
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<td>-1</td>
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<tr>
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<td>-1</td>
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<td>-1</td>
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<td>-1</td>
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<td>0</td>
<td>-1</td>
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<td>-1</td>
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<td>1</td>
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<tr>
<td>1</td>
<td>-1</td>
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<td>-1</td>
<td>0</td>
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<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>1</td>
<td>0</td>
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<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

The estimates of the un-standardized parameters are $\hat{\beta}_0 = 9.18$, $\hat{\beta}_1 = -0.8625$, $\hat{\beta}_2 = -0.06$, $\hat{\beta}_3 = 0.283$, $\hat{\beta}_4 = 0.01$, $\hat{\beta}_{22} = 0.852$, $\hat{\beta}_{11} = 0.1875$, $\hat{\beta}_{33} = 0.439$.
\( \hat{\beta}_{44} = 0.824 \), \( \hat{\beta}_{12} = -0.66 \), \( \hat{\beta}_{13} = -0.91 \), \( \hat{\beta}_{14} = -1.822 \), \( \hat{\beta}_{23} = 0.15 \), \( \hat{\beta}_{24} = -0.2275 \), and \( \hat{\beta}_{34} = -0.695 \). The variance of the estimated response is 2.1715. The proportion of variance indices corresponding to the parameters are \( s_0 = 0.33 \); \( s_1 = 0.083 \); \( s_2 = 0.083 \); \( s_3 = 0.083 \); \( s_4 = 0.083 \); \( s_{11} = 0.1875 \); \( s_{22} = 0.1875 \); \( s_{33} = 0.1875 \); \( s_{44} = 0.1875 \); \( s_{12} = 0.25 \); \( s_{13} = 0.25 \); \( s_{14} = 0.25 \); \( s_{23} = 0.25 \); \( s_{24} = 0.25 \); \( s_{34} = 0.25 \).