International Journal of Mathematics and Statistics Invention (IJMSI)
E-ISSN: 2321 – 4767 P-ISSN: 2321 - 4759
www.ijmsi.org Volume 3 Issue 5 || July. 2015 || PP-01-05

Estimation of Parameters and Missing Responses In Second Order Response Surface Design Model Using Em Algorithm

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Summary : *This article is an attempt to explore missing responses in second order response design model using Expected Maximization algorithm with and without imposing restrictions on the design matrix towards or thogonality are derived and are implemented with suitable examples. The properties of estimated parameters and estimated responses are also studied and findings are presented in detail at the end of the study.*

Keywords : *EM algorithm, Estimation of Missing responses, Second Order Response Surface Design Model*

I. INTRODUCTION

Let X = ($X_1, X_2, \ldots, X_v$) be the vector of v factors, each factor with 's' levels for experimentation and let x_{ui} be the level of the i^{th} factor in the u^{th} treatment combination (i=1,2 ... v; u =1,2…N) and let D_{Nxv} = ((x_{u1}, x_{u2} … x_{uv})) denotes the design matrix of the combination of the factor levels. Let Y_u denotes the response at the u^{th} combination. The factor-response relationship is given by $E(Y_u) = f(x_{u1}, x_{u2} \ldots x_{uv})$ is called the 'response surface'. The functional form of the response surface may be first order, second order…etc. The design used for fitting the response surface model is termed as 'response surface design' and the model is called 'response surface design model'. Suppose it is required to fit a second order response surface design model expressed in the form

$$\underline{Y} = X\underline{\beta} + \underline{\varepsilon} \tag{1.1}$$

Where $\underline{Y} = (Y_1, Y_2 \ldots Y_N)'$ is the vector of responses,

$X_u = (1, x_{u1}, x_{u2} \ldots x_{uv}, x^2_{u1}, x^2_{u2} \ldots x^2_{uv}, x_{ul}x_{u2} \ldots x_{uv-1}x_{uv})$ is the u^{th} row of X,

$\underline{\beta} = (\beta_0, \beta_1, \beta_2 \ldots \beta_v, \beta_{11}, \beta_{22} \ldots \beta_{vv}, \beta_{l2} \ldots \beta_{v-1v})'$ is the vector of parameters.

$\underline{\varepsilon} = (\varepsilon_1, \varepsilon_2 \ldots \varepsilon_N)$ is the vector of random errors and follows $N(0,\sigma^2 I)$.

Least square estimate of parameters is $\hat{\beta} = (X'X)^{-1}X'Y$ with $Var(\hat{\beta}) = (X'X)^{-1}\sigma^2$, where, $X'X = \begin{bmatrix} N & [j] & [jj] & [jk] \\ [i] & [ij] & [ijj] & [ijk] \\ [ii] & [iij] & [iijk] & [iijk] \\ [ij] & [[ijj] & [ijjj] & [ijjk] \end{bmatrix}$; where [i], [ij], [ijk], [ijkl] are terms related to sum of design levels of factor(s) $\boldsymbol{x}_{ui}$, $\boldsymbol{x}_{ui}\boldsymbol{x}_{uj}$, $\boldsymbol{x}_{ui}\boldsymbol{x}_{uj}\boldsymbol{x}_{uk}$, $\boldsymbol{x}_{ui}\boldsymbol{x}_{uj}\boldsymbol{x}_{uk}\boldsymbol{x}_{ul}$ over the N design points. Then the estimated value of the response at the u^{th} design point is

$$\hat{Y}_u = \hat{\beta}_0 + \sum_{i=1}^{v} \hat{\beta}_i \boldsymbol{x}_{ui} + \sum_{i=1}^{v} \hat{\beta}_{ii} \boldsymbol{x}_{ui}^2 + \sum_{i<j}^{v} \hat{\beta}_{ij} \boldsymbol{x}_{ui} \boldsymbol{x}_{uj} \tag{1.2}$$

Suppose the restrictions imposed on the moment matrix X'X towards reaching to orthogonality for a second order response surface design model are $\sum_{u=1}^{N} x_{ui}^{\delta_i} x_{uj}^{\delta_j} x_{uk}^{\delta_k} x_{ul}^{\delta_l} = 0$; i≠j≠k≠l=1,2… v for any δ value is odd and $\sum_{u=1}^{N} x_{ui}^2 = N\lambda_2$; $\sum_{u=1}^{N} x_{ui}^4 = cN\lambda_4$; $\sum_{u=1}^{N} x_{ui}^2 x_{uj}^2 = N\lambda_4$ and let $\Delta = \lambda_4(C+v-2)-v\lambda_2^2 > 0$. Then the moment matrix X'X and $(X'X)^{-1}$ can be obtained as

$$X'X = \begin{bmatrix} 1 & 0 & \lambda_2 J & 0 \\ 0 & \lambda_2 I & 0 & 0 \\ \lambda_2 J & 0 & [(c-1)I+J]\lambda_4 & 0 \\ 0 & 0 & 0 & \lambda_4 I \end{bmatrix}; \quad (X'X)^{-1} = \begin{bmatrix} \lambda_4(c+k+1)\Delta^{-1} & 0 & (c+k-1)(c-1)J\Delta^{-1} & 0 \\ 0 & \lambda_2^{-1} I & 0 & 0 \\ -2\lambda_2 J\Delta^{-1} & 0 & Z & 0 \\ 0 & 0 & 0 & \lambda_2^{-1} \end{bmatrix} \tag{1.3}$$

Where $\Delta = \lambda_4 (c+k-1) - k\lambda_2^2 > 0$ and $Z_{kxk} = \frac{[(c+v-1)I_v - J_{v,v}]}{\lambda_4(c-1)(c+v-1)} + \frac{[\lambda_2^2(c+v-1)(c-1)^2]}{[\lambda_4(c+v-1)-k\lambda_2^2]} J_{k,k}$

if any set of observations miss, in well-planned experiments the resulting data is incomplete to carry out the analysis as per the original plan. For these contexts Yates (1933) developed an iterative process starting with some initial guessing values. Healy and Westmacott (1956) described a more general iterative method for estimating the missing values. Draper N.R (1961), et.al, made attempts on the estimation of missing values in design and analysis of experiments.

II. EXPECTED MAXIMIZATION ALGORITHM

Let $\underline{\mathbf{y}} = [\, y_1, y_2, y_3, \dots, y_n\,]'$ be the vector of observed sample of size 'n' corresponding at design points X. Let us assume that sample drawn from population with a Normal density function $\boldsymbol{f(y)}$ and the data may contain some unobserved or latent variable and unknown parameters. Let **L($\underline{y}$)** be the likelihood function and **log L($\underline{y}$)** be the log of likelihood function of the sample. Initially estimate the values of the parameters by maximizing the likelihood function based on the known observed sample. The expected value of log of likelihood function is evaluated. Based on the existing parameter the improved version of the parameter that maximizes the expected value of Log of Likelihood function can be evaluated by repeating the above two steps of evaluations until two successive iterations will results same value or with negligible difference.

There is a little review on the estimation of missing values in the experimental design using expected maximization algorithm directly. So an attempt is made to develop the procedure to estimate the parameters and missing responses for second order response surface design model using expected maximization algorithm.

III. ESTIMATION OF PARAMETERS AND MISSING RESPONSES IN RESPONSE SURFACE DESIGN MODEL USING EM ALGORITHM

Let $\underline{\mathbf{y}} = [y_1, y_2 \dots y_n]'$ be the vector of responses correspondingly at the design matrix $X_{nx(v+1)}$. Assume the factor-response relationship is linear with first order response surface model in v factors, satisfying the model (1.3). Assume the response variable Y follows Normal with E(Y) = Xβ with V(Y) = σ^2. Let us assume that the responses miss at some design points. Then the model (1.3) can be expressed as follows

$$\begin{bmatrix} Y_1 \\ Y_m \end{bmatrix} = \begin{bmatrix} X_1 \\ X_m \end{bmatrix} \beta + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_m \end{bmatrix} \tag{3.1}$$

where $\underline{Y}_1$ is the vector of (n-m) known observations, $\underline{Y}_m$ is the vector of 'm' missing observations, X_1 is part of the design points corresponding to the known and X_m is corresponding to the missing observations design points. Let the error is also partitioned accordingly. The least square estimate of the parameters from the known observations is $\hat{\beta} = (X_1' X_1)^{-1} X'_1 Y_1$. Then the estimated missing observations can be obtained as $\hat{Y}_m = X_m \hat{\beta}$.

Let us consider the problem of estimating the parameters and missing responses using expected maximization algorithm, then the response variable Y follows N(Xβ, σ^2). If $\underline{\mathbf{y}} = [y_1, y_2 \dots y_n]'$ be the observed responses (including missing responses) then the log of the likelihood function is

$$L(\underline{y}) = (2\pi\sigma^2)^{-n/2} \times \exp\left\{ \frac{-1}{2\sigma^2} \left[\sum_{j=1}^{n-m} (y_j - x_j\beta)^2 + \sum_{j=n-m+1}^{n} (y_j - x_j\beta)^2 \right] \right\} \tag{3.2}$$

$$\text{Log } L(\underline{y}) = -\frac{n}{2}\log 2\pi - \frac{n}{2}\log\sigma^2 - \frac{1}{2\sigma^2}\left[\sum_{j=1}^{n-m} (y_j - x_j\beta)^2 + \sum_{j=n-m+1}^{n} (y_j - x_j\beta)^2 \right] \tag{3.3}$$

The estimates of parameters β and σ^2 and missing responses (y_u ; u = n-m+1, … , n) can be obtained using maximum likelihood method as

$$\frac{\partial}{\partial\beta}\log L(y) = 0 \Rightarrow \hat{\beta} = \left[\sum_{j=1}^{n-m} x_j' x_j + \sum_{j=n-m+1}^{n} x_j' x_j \right]^{-1} \left[\sum_{j=1}^{n-m} x_j' y_j + \sum_{j=n-m+1}^{n} x_j' y_j \right] \tag{3.4}$$

$$\frac{\partial}{\partial\sigma^2}\log L(y) = 0 \Rightarrow \hat{\sigma}^2 = \frac{1}{n}\left[\sum_{j=1}^{n-m}(y_j - x_j\hat{\beta})^2 + \sum_{j=n-m+1}^{n}(y_j - x_j\hat{\beta})^2\right] \quad (3.5)$$

$$\frac{\partial}{\partial y_u}\log L(y) = 0 \Rightarrow \hat{y}_u = x_u\hat{\beta} \quad (3.6)$$

From the expectation of log of likelihood, the conditional expectation of missing observations can be obtained as

E [log L(y)] $\Rightarrow$ E $[y_u / y, X) = x_u \hat{\beta}^{(k)}$ and E $[y_u^2 / y, X) = (x_u \hat{\beta}^{(k)})'(x_u \hat{\beta}^{(k)}) + \sigma^{2(k)}$ (3.7)

From the equation (3.4), (3.5) and (3.6) and (3.7), by starting with initial guess values for missing observations, the recurrence equations can be obtained as

$$\hat{\beta}^{(k+1)} = [X'X]^{-1}\left[\sum_{j=1}^{n-m}x_j{}'y_j + \sum_{j=n-m+1}^{n}x_j{}'y_j{}^{(k)}\right] \quad (3.8)$$

$$\hat{\sigma}^{2(k+1)} = \frac{1}{n}\left[\sum_{j=1}^{n-m}(y_j - x_j\hat{\beta}^{(k+1)})^2 + \sum_{j=n-m+1}^{n}(y_j - x_j\hat{\beta}^{(k+1)})^2\right]$$

$$\Rightarrow \quad \hat{\sigma}^{2(k+1)} = \frac{1}{n}\left[(n-m)\hat{\sigma}_1^{2\,(k+1)} + m\hat{\sigma}_2^{2\,(k+1)}\right] \quad (3.9)$$

$$\hat{y}_u{}^{(k+1)} = x_u\hat{\beta}^{(k+1)} \quad (3.10)$$

The missing response values are assumed as zeros or average of known responses or arbitrary values and estimate β as $\hat{\beta} = (X'X)^{-1}X'Y$ and maximize the estimated response $\hat{Y}_m = X_m\hat{\beta}$ repeatedly maximize the estimated values for the parameters and missing responses until the values are stabilized.

Estimate β and Y_m vectors iteratively using (3.8) and (3.10) as $\hat{\beta} = (X_m'X_m + X_1'X_1)^{-1}(X_m'\hat{Y}_m + X_1'Y_1)$ and $\hat{Y}_m = X_m\hat{\beta}$. Assume missing response values as zeros or average of known responses or any arbitrary value. Iteratively maximize the estimated values using the same for the parameters and missing response values until the values are stabilized.

a. Assume missing response values as zeros and estimate β, its first iterative estimate is $\tilde{\beta}^{(1)} = (X'X)^{-1}(X_m'\mathbf{0}_m + X_1'Y_1) = (X'X)^{-1}X'Y$.
b. Assume missing response values as average of known responses and estimate β, its first iterative estimate is $\bar{\beta}^{(1)} = (X'X)^{-1}[X_m'\bar{Y}_{N-m} + X_1'Y_1] = (X'X)^{-1}X'Y$.
c. Assume missing response values as an arbitrary value and estimate β, its first iterative estimate is, $\ddot{\beta}^{(1)} = (X'X)^{-1}(X_m'A + X_1Y_1) = (X'X)^{-1}X'Y$.

The method of estimating the parameters and missing values using least square and EM algorithm (with initial guess values means and zeros) are implemented with suitable examples in case of second order response surface design under with and without restrictions on the moment matrix.

Example 3.1: Consider three factors of second order response surface design model with eighteen responses : 2.83, 3.25, 3.56, 2.53, 3.01, 3.19, $\mathbf{Y_7}$, 2.65, 3.06, 2.57, $\mathbf{Y_{11}}$, 3.50, 2.42, 2.79, 3.03, 2.07, 2.85, 3.12 at the design points (-1, -1, -1), (0, -1, -1), (1,-1, -1), (-1, 0, -1), (0, 0, 1), (1, 0, 1), (-1, 1, 1), (0, 1, 1), (1, -1, 0) (-1, -1, 0), (0, -1, -1), (1, 0, -1), (-1, 0, 1), (0, 0, -1), (1, 1, 0), (-1, 1, 1), (-1, -1, -1), (-1, 1, -1) respectively.

Let us consider the initial guess missing response values as $Y_7 = Y_{11} = 2.901875$ (average of known responses), and are zeroes , the estimated parameters and missing responses are evaluated using (3.8) - (3.10) and are same irrespective of iterations. And, if the initial guess missing values are taken as zeroes, the iterations are more (19 iteration) when average (16 iteration) is considered. The estimated values are $\hat{\beta}$ =[2.04114 0.45262 -0.23045 -0.04153 -0.01109 0.55668 0.87291 0.18637 -0.06678 -0.54492] and $\hat{Y}_{(-1, 1, 1,)}$= 2.080646, $\hat{Y}_{(0, -1, -1)}$= 3.207924.

The estimated values of missing responses using Least square method using the equations $\hat{Y}_u = X_u\hat{\beta}$ where $\hat{\beta} = (X_1'X_1)^{-1}X_1'Y_1$ as $\hat{\beta}$ = [2.04114 0.45262 -0.23045 -0.04415 -0.01109 0.55668 0.87291 0.18637 -0.06678 -0.54492] and $\hat{Y}_{(-1\ 1,\ 1,\ )}$= 2.080646, $\hat{Y}_{(0,\ -1,\ -1)}$= 3.207924

EXAMPLE 3.2: Consider a four factor second order response design model but not rotatable with 20 responses 63.03, 62.19, 64.01, 61.60, 58.95, Y_6, 45.75, 72.66, 46.36, 68.62, 35.16, 59.24, Y_{13}, 84.01, 61.18, 77.78, 61.15, 74.85, 52.45, 65.72 with the design points (0, 0, 0, 0), (0, 0, 0, 0), (0, 0, 0, 0), (0, 0, 0, 0), (-1,-1,-1,-1), (1,-1,-1,-1), (-1,1,-1,-1), (1,1,-1,-1), (-1,-1,1,-1), (1,-1,1,-1), (-1,1,1,-1), (1,1,1,-1), (-1,-1,-1,1), (1,-1,-1,1), (-1,1,-1,1), (1,1,-1,1), (-1,-1,1,1), (1,-1,1,1), (-1,1,1,1), (1,1,1,1) respectively.

Let us consider the initial guess missing response values as $Y_6 = Y_{13}$ =61.927222 (average of known responses), and are zeroes , the estimated parameters and missing responses are evaluated using (3.8) - (3.10) and are same irrespective of iterations. And, if the initial guess missing values are taken as zeroes, the iterations are more (48 iteration) when average (42 iteration) is considered. The estimated values are $\hat{\beta}$ = [62.707500 9.626248 4.802500 -5.603750 4.888750 0.209375 0.209375 0.209375 0.209375 0.481251 -0.465000 -2.475000 0.003750 0.651250 0.707500] and $\hat{Y}_{(-1,\ -1,\ -1,\ -1)}$ =82.50999, $\hat{Y}_{(-1,\ -1,\ -1,\ 1)}$ = 70.35001

The estimated values of missing responses using Least square method as $\hat{\beta}$ = [62.707500 9.626248 4.802500 -5.603750 4.888750 0.209375 0.209375 0.209375 0.209375 0.481251 -0.465000 -2.475000 0.003750 0.651250 0.707500] and $\hat{Y}_{(-1,\ -1,\ -1,\ -1)}$ =82.50999, $\hat{Y}_{(-1,\ -1,\ -1,\ 1)}$ = 70.35001

EXAMPLE 3.3: Consider a four factor second order rotatable design model with 27 responses 11.28, 8.44, $Y_{3,}$ 7.71, 8.94, 10.9, 11.85, 11.03, 8.26, 7.87, 12.08, 11.06, 7.98, 10.43, 10.14, 10.22, 10.53, $Y_{20,}$ 10.98, 9.56, 8.78, 9.02, 11.64, 8.24, 9.79 with the design points (-1, -1, 0, 0), (1,-1, 0, 0), (-1, 1, 0, 0), (1, 1, 0, 0), (0, 0, -1, -1), (0, 0, 1, -1), (0, 0, -1, 1), (0, 0, 1, 1), (0, 0, 0, 0), (-1, 0, 0, -1), (1, 0, 0, -1), (-1, 0, 0, 1), (1, 0, 0, 1), (0, -1, -1, 0), (0, 1,-1,0), (0, -1, 1, 0), (0, 1,1,0), (0, 0, 0, 0), (0, -1, 0, -1), (0, 1, 0, -1), (0, -1, 0, 1), (0, 1, 0, 1), (-1, 0, -1, 0), (1, 0, -1, 0), (-1, 0, 1, 0) ,(1, 0, 1, 0), (0, 0, 0, 0).

Let us consider the initial guess missing response values as $Y_3 = Y_{20}$ = 9.9014 (average of known responses), and are zeroes , the estimated parameters and missing responses are evaluated using (3.8) - (3.10) and are same irrespective of iterations. And, if the initial guess missing values are taken as zeroes, the iterations are more (47 iteration) when average (40 iteration) is considered. The estimated values are $\hat{\beta}$ =[9.18333 -0.46524 -0.57786 0.28333 0.01298 -0.45196 0.33589 0.69768 0.90304 0.53179 -0.91 -1.8225 0.15 0.13179 -0.695] and $\hat{Y}_{(-1,\ 1,\ 0,\ 0)}$ =8.422857, $\hat{Y}_{(0,\ 1,\ 0,-1)}$ = 9.582857

The estimated values of missing responses using Least square method as $\hat{\beta}$ = [9.18333 -0.46524 -0.57786 0.28333 0.01298 -0.45196 0.33589 0.69768 0.90304 0.53179 -0.91 -1.8225 0.15 0.131785 -0.695] and $\hat{Y}_3$=8.422857, $\hat{Y}_{20}$=9.582857.

IV. PROPERTIES ON ESTIMATED PARAMETERS AND MISSING RESPONSES

The properties of the estimated parameters are presented below.

1. If the numbers of missing responses increase, the difficulty level for estimating the parameters and missing responses increase due to the increase of number of equations to be solved.
2. An iterative approach is preferred if the number of equations to be solved is more. In these situations EM algorithm can be used.
3. The rate of convergence of EM algorithm is second order convergence.
4. From the examples 3.1, 3.2 and 3.3 it can be noted that both the least square and EM algorithm give same result. But in the EM algorithm the number of iterations are depends on the initial guess values.
5. It can be noted that Yates (1933) general iterative process and Healy, et.al (1956) iterative procedures are giving similar results with EM algorithm.
6. **If** $\hat{\beta} = (X_1' X_1)^{-1} X_1' Y_1$ then $E[\hat{\beta}] = E[(X_1' X_1)^{-1} X_1' Y_1] = \beta$ i.e. it is an unbiased estimate.
7. **If** $\tilde{\beta} = (X' X)^{-1} X_1' Y_1$ then $E[\tilde{\beta}] = (X' X)^{-1} (X_1'X_1)\, \beta$ i.e. it is not an unbiased estimate.
8. **If** $\bar{\beta} = (X'X)^{-1} [\, X_m' \bar{Y}_{N-m} + X_1'Y_1\,]$ then $E[\bar{\beta}] = \beta$ i.e. it is an unbiased estimate

9. If β is estimated through different approaches as $\hat{\beta} = (X_1'X_1)^{-1} X_1'Y_1$, $\tilde{\beta} = (X'X)^{-1}X_1'Y_1$, $\overline{\beta} = (X'X)^{-1} [X_m' \overline{Y}_{N-m} + X_1'Y_1]$, the relationship between the parametric relation is: $\hat{\beta} = [I + (X'X)^{-1} X_m'\mathbf{M}X_m] \tilde{\beta}$ where $M = [I - X_m(X'X)^{-1}X_m]^{-1}$ and $\overline{\beta} = [(X'X)^{-1} X' \overline{Y}_{N-m}] + \tilde{\beta}$

10. If the estimate of β is $\hat{\beta} = (X_m'X_m + X_1'X_1)^{-1} [X_m' \hat{Y}_m + X_1'Y_1]$ for a full model in case of missing responses, and $\hat{Y}_m = X_m \hat{\beta}$ and $\hat{\beta} = (X_1' X_1)^{-1} X_1' Y_1$, the value of

$\Rightarrow \hat{\beta} = (X'X)^{-1} [X_m'(X_m (X_1'X_1)^{-1} X_1'Y_1) + X_1'Y_1]$

$\Rightarrow \hat{\beta} = (X'X)^{-1} [(X_m'X_m) (X_1'X_1)^{-1} X_1'Y_1 + X_1'Y_1]$

$\Rightarrow \hat{\beta} = (X'X)^{-1} [(X'X - X_1'X_1) (X_1'X_1)^{-1} + I] X_1'Y_1$

$\Rightarrow \hat{\beta} = (X'X)^{-1} [(X'X) (X_1'X_1)^{-1} - I + I] X_1'Y_1$

$\Rightarrow \hat{\beta} = (X'X)^{-1} [(X'X) (X_1'X_1)^{-1}] X_1'Y_1$

$\Rightarrow \hat{\beta} = (X_1'X_1)^{-1} X_1'Y_1$

11. If the estimate of β is $\hat{\beta} = (X_m'X_m + X_1'X_1)^{-1} [X_m' \hat{Y}_m + X_1'Y_1]$ for a full model in case of missing responses, and $\hat{Y}_m = X_m \hat{\beta}$ and $\hat{\beta} = (X' X)^{-1} X_1' Y_1$, the value of $\hat{\beta}$ is

$\hat{\beta} = (X'X)^{-1}[2I - (X'_1X_1) (X'X)^{-1}] X_1'Y_1$

12. In case of Central Composite Design or any other Response Surface Design, if the responses are miss at origin and the responses are known at all other points the estimated value of the parameter $\hat{\beta}$ will be same as $\hat{\beta} = (X'X)^{-1} X_1'Y_1 = (X'_1X_1)^{-1}X_1'Y_1$ because $X'_mX_m=0$

Acknowledgements: The authors are thankful to the UGC for providing the fellowship to carry out this research work under the BSR RFSMS scheme and also thankful to the referees for improving the manuscript.

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