Pak J Commer Soc Sci
Pakistan Journal of Commerce and Social Sciences
2013, Vol. 7 (1), 157-165

Alternative Approach to Fitting First-Order Model to the Response Surface Methodology

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Abstract

In this paper, we present the computational procedure of the First-Order Model in Response Surface Methodology (RSM) in a new dimension. Firstly, we fit the First-Order Model to a 2^k design by applying Yates' technique to calculate the sum of squares of main effects and their interactions. Secondly, we prove that SS regression and SS linear are equivalent. Thirdly, we give a new idea for computing SS quadratic under the concept of unbalanced Completely Randomized Design. The formula used in this technique is numerically and mathematically equivalent to the existing technique. Lastly, we split the total variation in the responses into all possible sources with the help of a diagram.

Keywords: Quadratic effect in response surface, first-order model, SS regression, SS linear.

1. Introduction

In RSM, we deal with the factorial design along with some central observations. In factorial design all possible combinations, of different factors each at same number of levels, are considered as treatments. The basic theory of experimental design includes the need of replication of original set of treatments to estimate the error present in the experiment which helps in testing the hypothesis whether treatments differ significantly from one another by comparing variation present between the treatments to the variation present within the treatments.

In RSM, treatments as defined above are not replicated because factorial experiment, itself, produces a large number of treatments to run. Without replication, method is unable to estimate the error of the experiment. This deficiency of the method is avoided by the inclusion of some central observations. In other words, we can say that treatments replicated at the centre provide an estimate for the error present in the experiment and also make it possible to test the higher order interactions. In RSM for First-Order Model, a 2^k factorial design is run to obtain the optimum response and the use of these central observations helps in indicating the presence of quadratic curve. First-Order Model includes linear regression analysis and detects the need of second-order model.

2. Literature Review

All the above concepts are being discussed below with the help of an example taken from *"Design and Analysis of Experiments" Classical and Regression Approaches with SAS* by Leonard C. Onyiah (2009).

Example states that yield of a chemical process is affected by three factors, the temperature, the time and the reactant concentration denoted by A, B and C respectively. Considering a 2^kfactorial experiment in which each factor is taken at 2 levels resulting in a set of 2^3= 8 observations. The levels for A, B and C are (40˚,48˚) ,(20,28) minutes and (10,18)% respectively. 5 observations are taken at the middle of the selected levels of each factor which are 44˚, 24 min and 14% respectively.

To analyze the linear regression model, the factors A, B and C are coded as -1, 0 and 1at low, medium and high levels and renamed as x_1,$x_2$and x_3 respectively.

Table 1: Results of the Chemical Process Experiment

Treatments	***A***	***B***	***C***	x_1	x_2	x_3	**Response y**	
(l)	40	20	10	-1	-1	-1	12.0	y_{if}
a	48	20	10	1	-1	-1	14.4	
b	40	28	10	-1	1	-1	10.8	
ab	48	28	10	1	1	-1	13.6	
c	40	20	18	-1	-1	1	10.4	
ac	48	20	18	1	-1	1	16.6	
bc	40	28	18	-1	1	1	9.0	
abc	48	28	18	1	1	1	16.0	
y_{1c}	44	24	14	0	0	0	13.0	y_{ic}
y_{2c}	44	24	14	0	0	0	11.8	
y_{3c}	44	24	14	0	0	0	13.6	
y_{4c}	44	24	14	0	0	0	12.0	
y_{5c}	44	24	14	0	0	0	13.2	

The First-Order Model is of the form:

$$y = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + \varepsilon \qquad (2.1)$$

In matrix form $y = Xb + \varepsilon$ where $b = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{bmatrix}$

b can be obtained as:

$$b = (X'X)^{-1} X'y$$

where $$X'y = \begin{bmatrix} \Sigma y \\ \Sigma x_1 y \\ \Sigma x_2 y \\ \Sigma x_3 y \end{bmatrix} = \begin{bmatrix} 166.4 \\ 18.4 \\ -4 \\ 1.2 \end{bmatrix}$$

As x_1, x_2 and x_3 are orthogonal to each other, the alternative relations can be used which are as under:

$b_0 = \Sigma y / n$, $b_1 = \Sigma x_1 y / \Sigma x_1^2$,
$b_2 = \Sigma x_2 y / \Sigma x_2^2$, $b_3 = \Sigma x_3 y / \Sigma x_3^2$.

Therefore

$$b' = [166.4/13 \;\; 18.4/8 \;\; -4/8 \;\; 1.2/8] \qquad (2.2)$$

The fitted First-Order Model is:

$$y = 12.8 + 2.3x_1 - 0.5x_2 + 0.15x_3 \qquad (2.3)$$

For ANOVA the following sums of squares are required.
SS total = 55.2

$$\text{SS regression} = b'X'y - (\Sigma y_i)^2/n \qquad (2.4)$$

SS regression

$$= [166.4/13 \;\; 18.4/8 \;\; -4/8 \;\; 1.2/8] \begin{bmatrix} 166.4 \\ 18.4 \\ -4 \\ 1.2 \end{bmatrix} - (166.4)^2/13 = 44.5$$

SS residual = SS total – SS regression = 10.7

SS residual can be partitioned into three Sums of Squares which are SS interaction, SS pure quadratic and SS pure error.

SS interaction

SS interaction = $SS_{12} + SS_{13} + SS_{23} + SS_{123}$
df = 4

where $SS_{12} = (\Sigma x_1 x_2 y)^2 / 2^3$
$SS_{13} = (\Sigma x_1 x_3 y)^2 / 2^3$
$SS_{23} = (\Sigma x_2 x_3 y)^2 / 2^3$
$SS_{123} = (\Sigma x_1 x_2 x_3 y)^2 / 2^3$

SS_{12}= 0.18 SS_{13}= 8
SS_{23} =0 SS_{123}=0.02
Therefore,
SS interaction = 8.2

SS pure quadratic

SS pure quadratic $= n_f n_c (\bar{y}_f - \bar{y}_c)^2 / (n_f + n_c)$ (2.5)

df = 1

n_f : number of observations in 2^3 factorial design. *i*.e. n_f = 8

n_c : number of observations obtained at the centre of the design. i.e. n_c = 5

$\bar{y}_f - \bar{y}_c$ indicates the existence of a quadratic effect.

SS pure quadratic= 0.052

SS pure error

SS pure error $= \Sigma y_{ic}^2 - (\Sigma y_{ic})^2 / n_c$ = 2.448.

df $= n_c - 1$ = 4

Table 2: ANOVA for First-Order Model Fitted to the Data

SOV	df	SS	MS	F
Regression	3	44.5	14.833	12.477*
Residual	9	10.7	1.189	
interaction	4	8.2	2.05	3.350
quadratic	1	0.052	0.052	0.085
pure error	4	2.448	0.612	
Total	12	55.2		

Further study is related to the path of the steepest ascent

3. Proposed Technique

In this technique, there is no change in the computation of SS total and SS pure error but SS regression (or SS linear) and SS interaction will be calculated by applying Yate's technique for computing SS main effects and their interactions.
SS quadratic will be computed under the concept of unbalanced CRD which is numerically and mathematically equivalent to the previously used method.

Consider the responses (y) of the experiment are divided into the two groups as:

Table 3: Two Groups of Responses (y)

Group I	y_{if}	12.0	14.4	10.8	13.6	10.4	16.6
		9.0	16.0				
Group II	y_{ic}	13.0	11.8	13.6	12.0	13.2	

$G = \sum y_{if} + \sum y_{ic} = 102.8 + 63.6 = 166.4$

SS total =55.2

Now apply Yate's method to the data, to calculate sum of squares of main effects and their interactions.

Table 4: Applying Yates Method to Data

Treat ments	y	C_1	C_2	C_3	**SS linear**	**SS interactions**
(l)	12	26.4	50.8	102.8		
a	14.4	24.4	52	18.4	$(18.4)^2/2^3$	
b	10.8	27.0	5.2	-4	$(-4)^2/2^3$	
ab	13.6	25.0	13.2	1.2		$(1.2)^2/2^3$
c	10.4	2.4	-2.0	1.2	$(1.2)^2/2^3$	
ac	16.6	2.8	-2.0	8.0		$(8)^2/2^3$
bc	9.0	6.2	0.4	0.0		$(0)^2/2^3$
abc	16.0	7.0	0.8	0.4		$(0.4)^2/2^3$

$b_0 = G / n = 166.4/13$

$b_1 = [A]/ 2^3 = 18.4/8$

$b_2 = [B]/ 2^3 = (-4)/8$

$b_3 = [C]/2^3 = 1.2/8$

With these computations, the fitted First-Order Model is the same as in equation (2.3).

3.1 SS linear

Now see SS linear under this technique produces the same result as SS regression.

SS linear = SSA + SSB + SSC (3.1)

$= (18.4)^2/2^3 + (-4)^2/2^3 + (1.2)^2/2^3$

$= 44.5$

SS residual = SS error = 10.7

3.1 SS Linear

Now see SS linear under this technique produces the same result as SS regression.

SS linear = SSA + SSB + SSC (3.1)

$= (18.4)^2/2^3 + (-4)^2/2^3 + (1.2)^2/2^3$

= 44.5

SS residual = SS error = 10.7

Table 5: ANOVA Table for Regression

SoV	df	SS	MS	F
regression/linear	3	44.5	14.833	12.477*
residual/ error	9	10.7	1.189	
Total	12	55.2		

Now we want to see how this error has been subdivided among different sources. The obvious sources are

(i) interactions (ii) pure error (introduced by the additional 5 values).

(i) SS interaction = SSAB + SSAC + SSBC + SSABC

$= (1.2)^2/2^3 + (8)^2/2^3 + (0)^2/2^3 + (0.4)^2/2^3 = 8.2$

SS pure error is the total variation of the additional observations i.e.it enters through the values of y_{ic} .

(ii) SS pure error $= (13)^2 + (11.8)^2 + (13.6)^2 + (12)^2 + (13.2)^2$

$- (63.6)^2/5 = 2.448$

3.2 Quadratic Effect / Lack of Fit

Table 6: Reconstruct of ANOVA

SoV	df	SS	MS	F
regression / linear	3	44.5	14.833	12.477*
residual/ error	9	10.7	1.189	
interaction	4	8.2		
pure error	4	2.448		
Total	12	55.2		

As we see that the error enters through two obvious sources but there is some hidden source that completes the desired SS error (i.e. 10.7) and makes adjustment for 1 df as well. This hidden source (due to lack of fit) may be the quadratic effect of factors, so

SS quadratic = SS error – (SS interaction + SS pure error)

= 0.052

3.3 Alternative Approach for SS quadratic

Now see SS quadratic under the new technique**.** It can be computed by the method of SS between groups or treatments as in unbalanced CRD.

SS quadratic=SS between=$(102.8)^2/8 + (63.6)^2/5 – (166.4)^2/13$

$= 0.052$ (see Table 3)

the formula can be expressed and simplified as:

SS quadratic = SS between

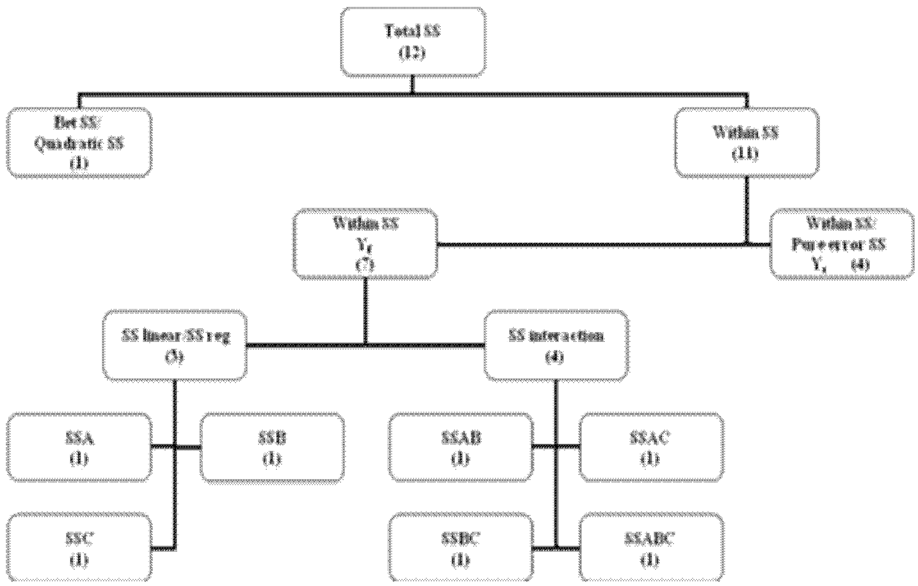
$$= (\sum y_{if})^2 / n_f + (\sum y_{ic})^2 / n_c - (G)^2 / (n_f + n_c) \qquad (3.2)$$

$$= (\sum y_{if})^2 / n_f + (\sum y_{ic})^2 / n_c - (\sum y_{if} + \sum y_{ic})^2 / (n_f + n_c)$$

3.4 Partitioning the Total Variation

A step by step partitioning of the total variation into several components along with their d.f can be made clearer with the help of the diagram below:

Diagram 1: Partitioning Total SS along with df



4. Comparison

Now see the comparisons of the two techniques below:

4.1 Comparison among Totals and entries in C_3.

Totals used in the calculations above and entries in column C_3 of Table 7 are equivalent.

Table 7: Comparison among Totals and entries in C_3

Treatments	**C_3**	**Comparison**
(l)	102.8	
a	18.4	$\sum x_1 y = 18.4$
b	-4	$\sum x_2 y = -4$
ab	1.2	$\sum x_1 x_2 y = 1.2$
c	1.2	$\sum x_3 y = 1.2$
ac	8	$\sum x_1 x_3 y = 8$
bc	0	$\sum x_2 x_3 y = 0$
abc	0.4	$\sum x_1 x_2 x_3 y = 0.4$

4.2 Comparison between the Results of (2.4) & (3.1)

See how SS regression in (2.4) and SS regression / SS linear in (3.1) match.
SS regression

$$= \begin{bmatrix} 166.4/13 & 18.4/8 & -4/8 & 1.2/8 \end{bmatrix} \begin{bmatrix} 166.4 \\ 18.4 \\ -4 \\ 1.2 \end{bmatrix} - \frac{(166.4)^2}{13}$$

$$= (166.4)^2/13 + (18.4)^2/8 + (-4)^2/8 + (1.2)^2/8 - (166.4)^2/13$$

$$= (18.4)^2/2^3 + (-4)^2/2^3 + (1.2)^2/2^3$$

$$= SSA + SSB + SSC \qquad (3.1)$$

$$= \text{SS linear}$$

Similarly, SS interactions for coded variables and SS interactions for actual variables are alike.

4.3 Mathematical Comparison

Now see that the mathematical expression, for SS quadratic/ SS between, introduced in (3.2) is mathematically equivalent to the previously used formula given in (2.5).
SS quadratic = SS between

$$= (\sum y_{if})^2/n_f + (\sum y_{ic})^2/n_c - (G)^2/(n_f + n_c) \qquad (3.2)$$

$$= (n_f \bar{y}_f)^2/n_f + (n_c \bar{y}_c)^2/n_c - (n_f \bar{y}_f + n_c \bar{y}_c)^2/(n_f + n_c)$$

$$= [(n_f \bar{y}_f)^2 n_c^2 + (n_c \bar{y}_c)^2 n_f^{\,2} - 2 n_f \bar{y}_f \, n_c \bar{y}_c\,]/n_f n_c (n_f + n_c)$$

$$= n_f n_c (\bar{y}_f - \bar{y}_c)^2/(n_f + n_c) \qquad (2.5)$$

6. Conclusion

The comparison shows how the proposed technique and previously used method go hand in hand by doing the analysis of the problem in a different perspective. The use of this technique makes the computational procedure more simple and easy. Further, the step by step partitioning of the total variation into all possible sources has been illustrated with the help of diagram to make the entire discussion conceptually more clear.

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