

Design and Analysis of Experiments
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Lecture – 56
Analysis of Second Order Response Surfaces

Welcome, we will discuss analysis of second order response surface. In last class I have shown you that how to fit second order response surface given the experimental data in this class we will revisit this for 5 minutes and then I will stay to go to the analysis part and it will take around 35 to 40 minutes of time.

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Contents

- Second Order Model - Introduction
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- An Example: Second Order Model
- References

Source: This lecture is prepared based on Chapter 11 of "Design and Analysis of Experiments" by D C Montgomery, Wiley, 8th Edition

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Introduction: Second Order Model


- When the experimenter is close to the optimum, first order model will not work
- An approximation of higher order model is needed. Often 2nd order approximation works.
- The objective is to find the optimum set of operating conditions for the x's
- The second order model with k factors is

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i < j} \beta_{ij} x_i x_j + \epsilon$$


- Intercept = 1
- MEs = k
- 2-IEs = ${}^k C_2$
- 3-IEs = ${}^k C_2$
- ...
- ...
- k-IEs = ${}^k C_k = 1$

k	1 st order model	2 nd order model*
2	1+2=3	1+2+2+1=6
3	1+3=4	1+3+3+3=10
4	1+4=5	1+4+4+6=15
5	1+5=6	1+5+5+10=21

*Ignoring 3rd and higher order interactions



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And the primary contents of this lecture is taken from the book written by Montgomery Design Analysis of Experiments. So, you have seen this slide in last class also, that the second order response surface will be like this; y equal to beta 0 plus i equal to 1 to k beta i x i, then the second order term, then the interaction term and error term will also be there and you have seen that when the number of k factors increases, the parameters also increases. Find these other things what we have discussed earlier also


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Analysis of the Second Order Response Surface


- Location of the stationary point
- Characterizing the response surface

Location of the Stationary Point:

- Find the levels of x_1, x_2, \dots, x_k that optimize the predicted response
- $\frac{\partial^2 y}{\partial x_1^2} = \frac{\partial^2 y}{\partial x_2^2} = \dots = \frac{\partial^2 y}{\partial x_k^2} = 0$ (where k is the total number of x)
- The point say $x_{1,0}, x_{2,0}, \dots, x_{k,0}$ is called the stationary point
- The stationary point could represent a point of maximum response, a point of minimum response, or a saddle point



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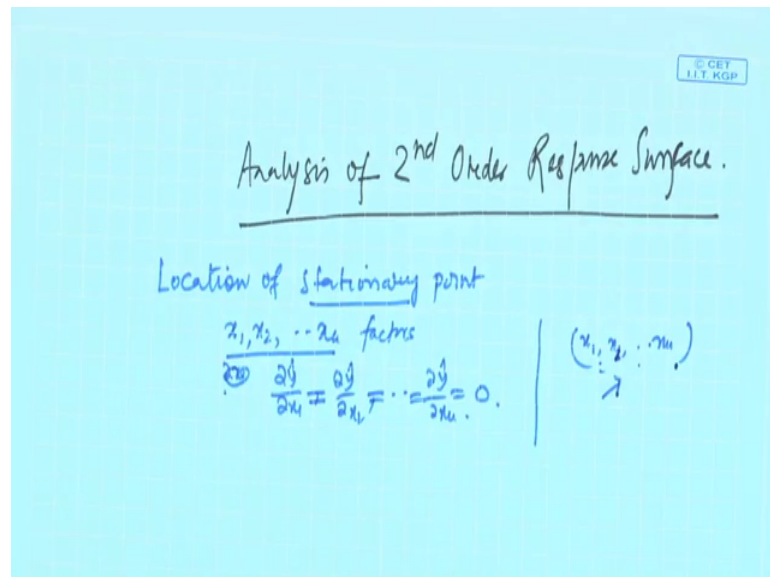


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Now, question is that, what are the issue that we should discuss when we talk about analysis of second order response surface. The second order response surface will be used to find out the optimum zone or settings for process operation or the system at

which, where should we operate the system or the process. So, that we will know that where is the location of the, where is the location of the maximum yield or maximum response, let such or minimum impurity that also minimum response something like this. So, first rule one is that you have to know location of stationary point.

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Stationary point means the point where the first derivative is equal to 0 ok. Suppose if we if we consider $x_1 \times x_2$ like x_k , these are the, these are the factors which basically define the design space, then $\frac{\partial y}{\partial x_1}$, sorry $\frac{\partial y}{\partial x_1}$ $\frac{\partial y}{\partial x_2}$. So, like this $\frac{\partial y}{\partial x_k}$; so this all, I think all will become 0 at the stationary point. So, then if $x_1 \times x_2 \times x_k$, suppose these are the factors, but at the same time if we say that the point $x_1 \times x_2$ then x_k , this is the point, because there are a k dimensions and there will be one point where values are $x_1 \times x_2 \times x_k$, let it be small $x_1 \times x_2 \times x_k$.

This is the point where the derivative, first derivative equal to 0, then this is a stationary point. So, you have to first find out the stationary point and then what is the nature of stationary point, whether it is a point of minimum or point of maximum or point of or a saddle point, where it is not sure point of maximum. It is not a point of maximum or minimum saddle point ok

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Location of Stationary Point

- Fitted second-order model in matrix notations $\hat{y} = \hat{\beta}_0 + x'b + x'Bx$

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} \quad b = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & \dots & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22} & \dots & \hat{\beta}_{2k}/2 \\ & & \dots & \vdots \\ \text{sym.} & & & \hat{\beta}_{kk} \end{bmatrix} \quad \frac{\partial \hat{y}}{\partial x} = b + 2Bx = 0$$

where $\hat{\beta}_i$ = Pure quadratic coefficient; $\hat{\beta}_{ij}$ = Mixed quadratic coefficient ($i \neq j$)

Stationary point: $x_s = -\frac{1}{2} B^{-1} b$

Predicted response at X_s : $\hat{y}_s = \hat{\beta}_0 + \frac{1}{2} x_s' b$

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Handwritten derivation of the stationary point for a second-order model:

$$y = \beta_0 + \sum \beta_i x_i + \sum \beta_{11} x_i^2 + \sum \sum \beta_{ij} x_i x_j + e$$

$$\hat{y}_s = \hat{\beta}_0 + \sum \hat{\beta}_i x_i + \sum \hat{\beta}_{11} x_i^2 + \sum \sum \hat{\beta}_{ij} x_i x_j$$

$$= \left(\hat{\beta}_0 + x_s' b + x_s' B x_s \right)$$

where $b = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix}$ and $B = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & \dots & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22} & \dots & \hat{\beta}_{2k}/2 \\ & & \dots & \vdots \\ \text{sym.} & & & \hat{\beta}_{kk} \end{bmatrix}$

$$\frac{\partial \hat{y}}{\partial x} = 0 + b + 2Bx = 0$$

$$x_s = -\frac{1}{2} B^{-1} b \quad \leftarrow \text{stationary point.}$$

Predicted stationary response: $\hat{y}_s = \hat{\beta}_0 + x_s' b + x_s' B (-\frac{1}{2} B^{-1} b)$

So, now let us see that how do we find out the point that location of stationary point and the related computation. This part is known to you. Now second order equation, when you estimate the beta then we write, these are all beta cap or beta hat. So, then the fitted value is y hat. So, y hat will be this portion except arrow term. So, this is what is y hat ok.

So, now, this one can be represented like this beta 0 cap cap plus x transpose b plus x transpose capital B x, where small b is the estimate of the first order coefficients, the beta

1 β_0 2 β_1 β_2 β_3 and capital B is basically it considered talking, it is basically con, it basically contains the second order that coefficient; that is quadratic part β_{11} β_{22} β_{33} and the interaction part like β_{12} β_{13} , β_{1k} and it will be half 1 by 2 1 by 2 and this side will be symmetry. So, ok

So, now if we consider that k equal to 2 that was considered k equal to 2, then your β_0 equal to β_0 and β_1 and your capital B equal to β_{11} , then β_{12} and then here again half half β_{12} and β_{22} cap, we all cap ok. So, this is what is capital B now. So, we can say that the point, the response surface is our fitted response surface is y cap equal to this and we say the location of stationary point is 1, where $\frac{\partial y}{\partial x}$ is 0.

So, $\frac{\partial y}{\partial x}$ equal to 0. So, if you take derivative with respect to x, then β_0 being the constant, its derivative will become 0 x transpose b derivative will be small b, and this quadratic term there will be 2 times b into x. So, we put equal to 0 and then you get the value of x, which is minus half B inverse b and this x is nothing, but the stationary point for x ok; so 2 b x equal to minus b so x equal to minus half B inverse b; that is the point, stationary point ok.

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$$\hat{y} = \beta_0 + \sum \beta_i x_i + \sum \beta_{ij} x_i x_j$$

$$= \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} + x' b + x' B x$$
 where $b = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}$ and $B = \begin{bmatrix} \beta_{11} & \frac{1}{2} \beta_{12} & \frac{1}{2} \beta_{13} \\ \frac{1}{2} \beta_{12} & \beta_{22} & \frac{1}{2} \beta_{23} \\ \frac{1}{2} \beta_{13} & \frac{1}{2} \beta_{23} & \beta_{33} \end{bmatrix}$ (symmetric)

$$\frac{\partial \hat{y}}{\partial x} = 0 + b + 2 B x = 0$$

$$x_s = -\frac{1}{2} B^{-1} b \leftarrow \text{stationary point.}$$

Predicted stationary response:

$$\hat{y}_s = \beta_0 + x_s' b + x_s' B (-\frac{1}{2} B^{-1} b)$$

$$= \beta_0 + x_s' b - \frac{1}{2} x_s' b = \beta_0 + \frac{1}{2} x_s' b$$

Then using this x s equal to these you will be able to find out that the predicted response at the stationary point will take, will be like this; that is β_0 half of x transpose b. So, if you want to derive it, derive it from the.

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$$\hat{y}_s = \beta_0 + x_s' b + x_s' B \left(-\frac{1}{2} B^{-1} b \right)$$

$$= \beta_0 + x_s' b - \frac{1}{2} x_s' b$$

$$= \beta_0 + \frac{1}{2} x_s' b$$

$$x_s = -\frac{1}{2} B^{-1} b$$

$$y = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \dots + \lambda_k w_k^2$$

$\lambda_1, \lambda_2, \dots, \lambda_k = \text{eigenvalue of Matrix } B$
 $w_1, w_2, \dots, w_k = \text{eigen-vector of Matrix } B$

All $\lambda > 0$ the point of min
 All $\lambda < 0$ " " " max
 Some $\lambda > 0, \lambda < 0$ — Saddle point

From the basic equation $\hat{y}_s = \beta_0 + x_s' b + x_s' B \left(-\frac{1}{2} B^{-1} b \right)$, there I will write minus half $B^{-1} b$ into x_s , because $x_s' x_s = \left(-\frac{1}{2} B^{-1} b \right)' \left(-\frac{1}{2} B^{-1} b \right)$. This we have seen, we have seen that at this equal to 0, x_s is equal to this.

Now in this formula we put $x_s = -\frac{1}{2} B^{-1} b$ and then you are getting like this. So, what is this, then this is $\beta_0 + x_s' b - \frac{1}{2} x_s' b$ and $B^{-1} b$ will be $-\frac{1}{2} B^{-1} b$. So, this is nothing, but the x_s is transfer b again. So, then this one is $\beta_0 + \frac{1}{2} x_s' b$. So, this is the predicted value at stationary point

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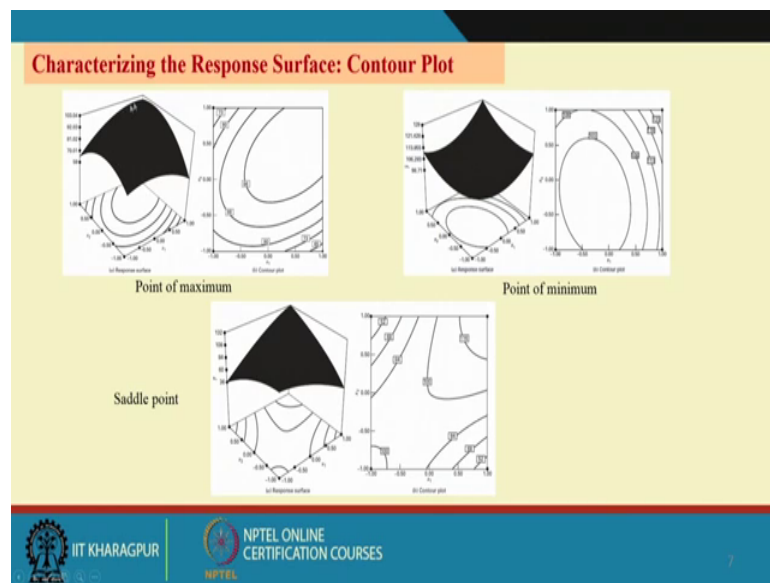
Characterizing the Response Surface

- By characterize, we mean determining whether a stationary point is (i) point of maximum, (ii) point of minimum, or (iii) saddle point
- Two methods are used
 - Contour plot of the fitted response (usually when $k \leq 3$)
 - Canonical analysis

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Now, we want to know whether this value is, and is the optimum value or not. So, in order to do; so you do one thing, either you go for contour plot of the fitted surface or canonical analysis, you do, because the stationary point can be a point of maximum, a point of minimum or a saddle point, determining whether the stationary point is a point of maximum point, a minimum or saddle point. So, that is done through two methods; one is contour plot another one is canonical analysis.

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So, let us see the contour plot. I have discussed contour plot several times earlier also when we have we have we have fitted the factorial experiments and then found out the regression equation and then the effect of x on the y through contour plot, we have explained several times. So, here, here you see, this is what is our response surface. So, here there are two variables in coded terms, we have written x_1 and x_2 plus minus 1 2 plus 1 minus 1 2 plus 1 and this is your response variable.

Now, if you see the contour plot, you see the contour plot. Contour plot mean, here it is the contour plot mean all the point on this line will have the same y response value. So, that mean here 96, then you have 88 then 80. So, if you go along this direction or the direction it is basically reducing. So, that mean this is the direction of improvement and somewhere here at the middle it will improve. So, this basically talks about, suppose this point which is somewhere here. So, this is point of maximum, because of this shape.

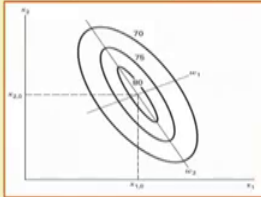
Now here what happen the shape says, this is valley or in this case point of maxima, saying it is a hill here, it is your valley and you are getting point to minimum also, but the third one if you see the contour plot, you move you go to one direction like this direction, then 100 and 116, here 100 then 84 68 52, here 84 60 52. So, it is, it is basically, it is difficult to tell that whether you are a point of maximum or point of minimum. So, it is a point which cannot be said either minimum or maximum. So, that is the helper.

So, contour plot will help you, but you know that contour plot is possible graphically for two dimensional or at mixed three dimensional case, when k equal to 3 or k equal to 2 or 3, but when k equal to more than 3, it is really difficult for all of us to use the contour plot, we require a better method of doing this work and that better method is known as Canonical Analysis

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Characterizing the Response Surface: Canonical Analysis

- Transform the fitted model into a new coordinate system with the origin at the stationary point (x_s) and the axes parallel to the principal axes of the fitted response surface



$$\hat{y} = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \dots + \lambda_k w_k^2 \rightarrow \text{Canonical form}$$

where $\{w_i\}$ are the transformed independent variables
 $\{\lambda_i\}$ are constants or the eigen values of the matrix B

$\lambda_i, i = 1, 2, \dots, k$	x_s is
All $\lambda_i > 0$	Point of minimum
All $\lambda_i < 0$	Point of maximum
Both +ve and -ve λ_i	Saddle point

$$B = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & \dots & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22} & \dots & \hat{\beta}_{2k}/2 \\ & & \dots & \\ \text{sym.} & & & \hat{\beta}_{kk} \end{bmatrix}$$

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What is the approach here in canonical analysis you see. So, this x_1 and x_2 , suppose these are the contour plots. So, at this and the inner ellipse that talks about the response of y equal to 80, then middle 175 and the outer one is 70. So, somewhere here the maximum or hill or maximum response lies. If you see the principal axis of the ellipses and the axis, axis of x_1 and x_2 , you see that they are not parallel. So, what in canonical analysis we want to do.

We want to first shift the 0 point to the center of the ellipse and then second we transform the x_1 and x_2 along, along that principal axis of the ellipse. So, you want to access like this, this one is one and another one is another w_1 and w_2 , which are parallel to the principal axis of the ellipse, not that parallel to x_1 and x_2 so you transform it. So, then what happened in the transformed dimension, your response that response predicted will become that response at the stationary point response, means predicted response at the stationary point plus $\lambda_1 w_1^2$ plus $\lambda_2 w_2^2$ plus $\lambda_k w_k^2$.

So, this is a special form which is a typical form, which is known as canonical form ok. So, originally we are here x_1 and x_2 , my new dimension is there w_1 and w_2 . Why you are doing like this? Because your ellipse, the response contours they are basically their principal axes are axes are parallel to parallel to that w_1 w_2 dot w_1 w_2 the two dimension parallel to the principal axis, we want that.

So, here then you first find out what is the predicted value here and then at the canonical part. So, your y cap will become y s cap plus $\lambda_1 w_1^2$ plus $\lambda_2 w_2^2$ plus $\lambda_k w_k^2$, where λ_1 λ_2 dot dot dot λ_k . These are basically like, this is basically. They are the Eigen value, Eigen value of matrix matrix capital B that you have already seen and w_1 w_2 w_k are the Eigen vector Eigen vector of matrix b

So, just seeing their λ values you are in a position to find out the. So, seeing the λ value you are in a position to find out this, whether the stationary point is a point, a minimum point of maximum or point of inflation or that is the saddle point. So, let me repeat here that you, once you do this. So, you are getting this then λ values also are there. λ s are basically Eigen value of b and w or ω s are Eigen vector of b. And then seeing the value of λ you will note you are in a position to tell whether the, whether the stationary point is point a maximum point of minimum or saddle point.

If all λ , all λ greater than equal to 0 then it is point of minimum. If all λ less than equal; sorry if all λ greater than 0 and all λ less than 0, this is point of maximum and if some λ , some λ greater than 0. So, other λ less than 0 then this is saddle point. So, this is much.

So, it is better, it is acceptable better model than the contour, because you can find out the all the Eigen values of b and, but just by seeing the eigen values very objectively you

are in a position to tell whether you have gone to the maximum point or minimum point or the, it is not neither of the two ok. Essentially what you require, you require the matrix b and that also we have seen earlier.

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Example (Experiment-1)

A chemical engineer is interested in determining the operating conditions that maximize the yield of a process. Two controllable variables influence process yield: reaction time and reaction temperature. The engineer is currently operating the process with a reaction time of 35 minutes and a temperature of 155°F, which result in yields of around 40 percent. Because it is unlikely that this region contains the optimum, she fits a first-order model and applies the method of steepest ascent.

Process Data for Fitting the First-Order Model				
Natural Variables		Coded Variables		Response
ξ_1	ξ_2	x_1	x_2	y
30	150	-1	-1	39.3
30	160	-1	1	40.0
40	150	1	-1	40.9
40	160	1	1	41.5
35	155	0	0	40.3
35	155	0	0	40.5
35	155	0	0	40.7
35	155	0	0	40.2
35	155	0	0	40.6

$$\hat{y} = 40.44 + 0.775x_1 + 0.325x_2$$

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So, with this background let us see the example, this example we have discussed in several classes.

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Example (Augmentation of first order design): Second-order RSM

The experimenter decides to augment a first-order design with enough points to fit a second-order model. She obtains **four observations** at $(x_1 = 0, x_2 = \pm 1.414)$ and $(x_1 = \pm 1.414, x_2 = 0)$. The complete experiment is shown in **Table 1**, and the design is displayed in **Fig. 1**. In this second phase of the study, two additional responses were of interest: the **viscosity** and the **molecular weight** of the product. The responses are also shown in **Table 1**. We will focus on fitting a quadratic model to the yield response y_1 .

Table 1						
Natural Variables		Coded Variables		Responses		
ξ_1	ξ_2	x_1	x_2	y_1 (yield)	y_2 (viscosity)	y_3 (molecular weight)
80	170	-1	-1	76.5	62	2940
80	180	-1	1	77.0	60	3470
90	170	1	-1	78.0	66	3080
90	180	1	1	79.5	59	3090
85	175	0	0	79.9	72	3480
85	175	0	0	80.3	69	3200
85	175	0	0	80.0	68	3410
85	175	0	0	79.7	70	3290
85	175	0	0	79.8	71	3500
82.07	175	1.414	0	78.4	68	3360
77.93	175	-1.414	0	75.6	71	3020
85	182.07	0	1.414	78.5	58	3630
85	167.93	0	-1.414	77.0	57	3150

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Now, in last class I have given you, shown that the C C D is used here and we have.

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Example: Second-order RSM (Contd.)

Table below contains the calculations of "sequential or extra sums of squares" for the linear, quadratic, and cubic terms in the model. On the basis of the small P-value for the quadratic terms, the **second-order model** is fitted to the yield response.

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	80062.16	1	80062.16		
Linear	10.04	2	5.02	2.69	0.1166
2FI	0.25	1	0.25	0.12	0.7350
Quadratic	17.95	2	8.98	126.88	<0.001 Suggested
Cubic	2.042E-003	2	1.021E-003	0.010	0.9897 Aliased
Residual	0.49	5	0.099		
Total	80090.90	13	6160.84		

"Sequential Model Sum of Squares": Select the highest order polynomial where the additional terms are significant.

2nd Order Regression equation: $Yield = 79.94 + 0.995x_1 + 0.515x_2 - 1.376x_1^2 - 1.001x_2^2 + 0.25x_1x_2$

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We have also got this, this one, the second order response surface this one. What is your second response surface for the example, example y.

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$$y = 79.94 + 0.995x_1 + 0.515x_2 - 1.376x_1^2 - 1.001x_2^2 + 0.25x_1x_2$$

$$\hat{\beta}_0 = 79.94$$

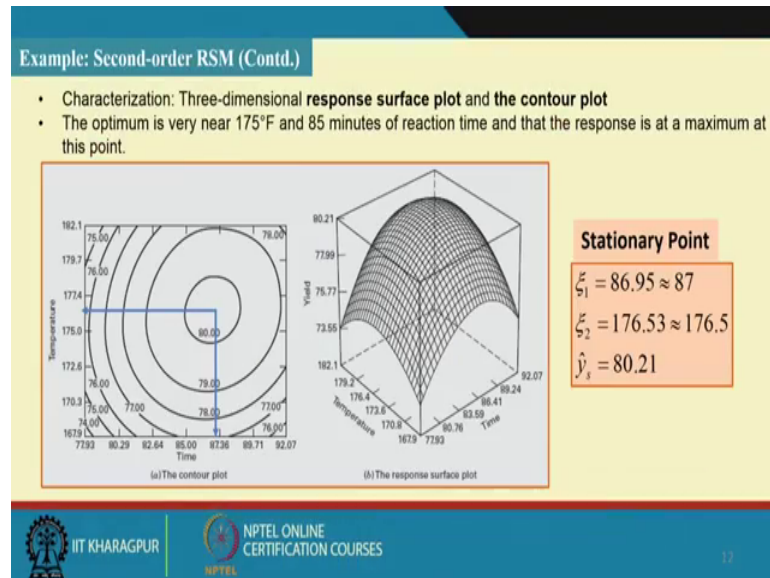
$$b = \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} \quad B = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12} \\ \hat{\beta}_{12} & \hat{\beta}_{22} \end{bmatrix} = \begin{bmatrix} -1.376 & 0.25 \\ 0.25 & -1.001 \end{bmatrix}$$

$$\hat{\beta}_0 = -79.94 + \frac{1}{2} \begin{bmatrix} 0.389 & 0.306 \end{bmatrix} \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix}$$

Which is, basically yield is 79.94 plus 0.995 x 1 plus 0.515 x 2 minus 1.376 x1 square minus 1.001 x2 square plus 0.25 x1 x2 ok. So, then what is this beta 0 is 79.94 then b, b is your 0.995 and 0.515 and capital B is what that beta 1 1 cap beta 2 2 cap half of beta 1 2 cap and half of beta 1 2 cap of here. So, this will be, what is beta 1 1 here.

Beta 1 1 means minus 1.376, what is beta 2 2? Beta 2 2 is minus 1.001, what is beta 1 2, beta 1 2 0.25. So, this is 0.25, but please remember there is a half so of diagonal element with half. So, this by 2 and this by 2, another minute B matrix will be minus 1.376 0.125 0.125 minus 1.00 1 2 cross 2. So, let us now analyze, let us now analyze this response surface using the methods that is known as canonical analysis.

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So, first one you see the contour plot then I will show you that you know. So, if you see the contour plot you are getting like this and here is the point; that is the point, stationary point and if you just project across this axis; that is time and this axis temperature. You are finding out the value, value for that time is around 87 and value for the temperature is around 167 76.5, and at this point what is the value of station yield is 80.21 and now ok. From this plot you are finding out this is, this is a point of maximum, because you see that the response surface is a hill like structure.

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Example: Second-order RSM (Contd.)

Location of the stationary point using the general solution given by $x_s = -\frac{1}{2} B^{-1} b$

$$b = \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} \quad B = \begin{bmatrix} -1.376 & 0.1250 \\ 0.1250 & -1.001 \end{bmatrix}$$



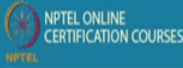

The stationary point:

$$x_s = -\frac{1}{2} B^{-1} b = -\frac{1}{2} \begin{bmatrix} -0.7345 & -0.0917 \\ -0.0917 & -1.0096 \end{bmatrix} \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} = \begin{bmatrix} 0.389 \\ 0.306 \end{bmatrix}$$

$$x_{1,s} = 0.389 \text{ and } x_{2,s} = 0.306 \quad (\text{Since, } 0.389 = \frac{\xi_1 - 85}{5} \text{ and } 0.306 = \frac{\xi_2 - 175}{5})$$

The natural variables:

$$\xi_1 = 86.95 \approx 87 \text{ and } \xi_2 = 176.53 \approx 176.5$$

$$\hat{y}_s = 80.21$$





Now, I want to, we want to use the canonical part. So, what is the stationary point x_s is minus half B inverse b . Now, b part is given to you. So, b part is, b part is small b is this and this one is this. So, what you require to do. You require to find out b inverse ok; so b inverse in to. So, what do you want half B inverse b ; that is minus of that is your x_s minus of B inverse b is x_s .

So, this value, this value when you compute, it will become 0.389 and 0.306. So, B is this, capital B is this, you find out the inverse of it multiplied divided by half minus symbol you use and then you will be getting you know. So, I mean this is the point x , this is the stationery point in terms of design variables, then what you want? You want y_s this value. So, what is the y_s value we have computed earlier? y_s value we have computed that y_s that is predicted y at s is β_0 plus half x inverse b , all those things are known to us

So, if you apply this one then β_0 is 79.94 plus half your stationary point, its transpose 0.389 0.306 and into b , what is your b point 0.995 and 0.515.

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So, this, this value is 80 point how much. It is a 80.21. So, you are getting one end. What is the stationary point, what is the predicted response? A stationary point right. Now what do you want whether this stationary point is a maximum point of maximum, because the contour chart says this is point of maximum.

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Example: Second-order RSM (Contd.)

Canonical analysis for characterizing the response surface

$$|B - \lambda I| = 0$$

$$\begin{vmatrix} -1.376 - \lambda & 0.1250 \\ 0.1250 & -1.001 - \lambda \end{vmatrix} = 0$$

$$\lambda^2 + 2.3788\lambda + 1.3639 = 0$$

$(\lambda_1 = -0.9634 \text{ and } \lambda_2 = -1.4141)$

$$\hat{y}_1 = \hat{\beta}_0 + \frac{1}{2}x_1'b$$

$$\frac{1}{2}x_1'b = \frac{1}{2} [0.389 \quad 0.306] \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} = 0.2723$$

$$\hat{\beta}_0 = \frac{79.9 + 80.3 + 80.0 + 79.7 + 79.8}{5} = 79.94$$

$$\hat{y}_1 = 80.21$$

Coded Variables		
x_1	x_2	y_1 (YMM)
-1	-1	76.5
-1	1	77.0
1	-1	78.0
1	1	79.5
0	0	79.9
0	0	80.3
0	0	80.0
0	0	79.7
0	0	79.8
1.414	0	78.4
-1.414	0	75.6
0	1.414	78.5
0	-1.414	77.0

Canonical form of the fitted model $\rightarrow \hat{y} = 80.21 - 0.9634w_1^2 - 1.4141w_2^2$ (Since $\lambda_1 = -0.9634$ and $\lambda_2 = -1.4141$)

Key Finding: $\hat{y} = \hat{\beta}_0 + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \dots + \lambda_n w_n^2$

Because both λ_1 and λ_2 are negative and the stationary point is within the region of exploration, we conclude that the stationary point is a maximum.

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$$|B - \lambda I| = 0$$

$$\begin{vmatrix} -1.376 & 0.125 \\ 0.125 & -1.001 \end{vmatrix} - \lambda \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} = \begin{vmatrix} -1.376 - \lambda & 0.125 \\ 0.125 & -1.001 - \lambda \end{vmatrix}$$

$$\lambda^2 + 2.3788\lambda + 1.3639 = 0$$

Roots:

$$\lambda_1 = -0.9634$$

$$\lambda_2 = -1.4141$$

So, in order to do, so what do you require? You require to find out B minus lambda i determinant equal to 0 to get the Eigen value and Eigen vector and your B is minus 1.376 0.125 0.125 minus 1.001, this minus lambda 1001. So, this is what is b minus lambda i equal to minus 1.376 minus lambda 0.125 0.125 minus 1.001 minus lambda. So, this is my matrix ok

So, now you take the determinant and then the determinant of these determinant of this. This will give you the equation called lambda square plus 2.37 8 8 lambda plus 1.3639, this put equal to 0, this you put to 0 and then find out that the roots, find out the roots of this equation lambda 1 and lambda 2. So, lambda 1 minus 0.9634 and this one is 1.4141 ok. So, now, you know you have lambda 1. So, now, all lambda 1, lambda values are negative. So, this is a point of maximum. Once you know the lambda values you know whether point of maximum or minimum is reached or it is a saddle point ok

Now, come back to this. So, both, because both lambda 1 and lambda 2 are negative and the stationary point is within the region of exploration. We conclude that the stationary point is a maximum canonical form of the fitted model. Now here we have shown that how beta 0 is calculated; that is the average value at the center point fine.

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Example: Second-order RSM (Contd.)

Finding the relationships between canonical variables and design variables:

Canonical variables = $\{w_i\}$
 Design variables = $\{x_i\}$

- Many a times, we could not operate the process at stationary point because this combination of factors may result in excessive cost.
- We require to move from the stationary point to a point of lesser cost without incurring large losses in response
- The canonical form of the model indicates the direction less sensitive to loss
- Exploration of the canonical form requires converting points in the (w_1, w_2) space to points in the (x_1, x_2) space.

x is related to w by the equation $w = M'(x - x_0)$ (where M is $(k \times k)$ orthogonal matrix)

$(B - \lambda_i I)m_i = 0$ (For which $\sum_{j=1}^k m_{ij}^2 = 1$, and m_i is the i -th column of M)

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Now, now what happened when we could not operate the process at the stationary point? So, many a times we could not operate the process at stationary point, because this combination of factors may result in excessive cost. We required to move from the stationary point to a point of lesser cost without incurring large losses in response, the canonical form of the model indicates the direction of less sensitive to loss exploration of the canonical forms requires converting points in the w_1 w_2 space to the point in the x_1 and x_2 space, what is happening here. Let us see.

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$\hat{y} = \hat{y}_s + \lambda_1 w_1 + \lambda_2 w_2$

$(w_1, w_2) \rightarrow (x_1, x_2)$

Approach
 Propose
 Methods of Steepest
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So, you have seen that. So, our stationary point is this and then this one is w_1 and this is the w_2 axis, and suppose your response surface your contour plots are like this. Suppose you would not operate here, because maybe cost is prohibitive or the technicalities is a problem for operators point of view or something, something like this. So, then what happened, you want another point another location another zone, where you will operate the process, you will not incur much loss at the same time, it will become convenient to do it.

So, that is possible, because you know that the directions x_1 w_1 and w_2 and you know that which direction if you go. If you go to the direction, what is the loss, minimum loss will be in which then directional direction that also known to you, because you know the function, you know the y cap in with in terms of y s stationary point plus $\lambda_1 w_1^2$ plus $\lambda_2 w_2^2$ we. They go along this diamond selection or the direction or depends on the value of λ will direction, you will incur less loss

So, this is one advantage of having this. Now second is that ok, suppose you will you will go along w_1 , because λ_1 is giving you better situation then question is that, you know those in w_1 and w_2 dimension, but you have to experiment it. So, you have to convert back to x_1 and x_2 ; so w_1 and x_1 . So, w_1 and w_2 , this dimensions it should be, this must be relation with x_1 and x_2 dimension, this how do you know.

So, there is, there is the concept called, there is a concept called, this w is related with x with this equation w equal to $M^T x - x_s$, where M is basically a orthogonal matrix and it is k cross k dimensions, because we have k number of factors, then this ultimately leads to this $b - \lambda_i = 0$

Now, you already know the λ values put λ_1 and then find out the m_i value, put another λ , find out the M value and then what happened. Once you know this m_i ; that means, m the M^T is known. Now using these equations you will get the relations between x m ω .

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Example: Second-order RSM (Contd.)

For $\lambda_1 = -0.9634$

$$(\mathbf{B} - \lambda_1 \mathbf{I}) \mathbf{m}_1 = \mathbf{0} \Rightarrow \begin{bmatrix} (-1.376 + 0.9634) & 0.1250 \\ 0.1250 & (-1.001 + 0.9634) \end{bmatrix} \begin{bmatrix} m_{11} \\ m_{21} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

We know that $\mathbf{b} = \begin{bmatrix} 0.800 \\ 0.533 \end{bmatrix}$, $\mathbf{B} = \begin{bmatrix} -1.376 & 0.1250 \\ 0.1250 & -1.001 \end{bmatrix}$

$$\begin{aligned} -0.4129m_{11} + 0.1250m_{21} &= 0 \\ 0.1250m_{11} + 0.0377m_{21} &= 0 \end{aligned}$$

$$\sqrt{(m_{11}^*)^2 + (m_{21}^*)^2} = \sqrt{(0.3027)^2 + (1)^2} = 1.0448$$

(Since, $\sum_{j=1}^k m_{ij}^2 = 1$; $m_{i1}^* = 1$, and $m_{i1}^* = 0.3027$)

Normalized solutions: $m_{11} = \frac{m_{11}^*}{1.0448} = \frac{0.3027}{1.0448} = 0.2898$ $m_{21} = \frac{m_{21}^*}{1.0448} = \frac{1}{1.0448} = 0.9571$

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This is what we are doing here. We know \mathbf{b} , we know λ . Now you put the first one what is the; so minus this into this value. So, minus is there minus plus minus is minus minus is plus. So, your resultant matrix is this and it is multiplied with m_{11} and m_{21} , because your head is the two dimensional case, then you are getting these two equations. Now these two equations wants you and two unknowns. So, you can solve it, but you will get a situation, where you find out that you will get infinite number of. So, an unique solution you will not get here, and as a result you require to normalize it.

The normalization one is this $\sum_{j=1}^k m_{ij}^2 = 1$ to k $m_{ij}^2 = 1$. So, that is what we have done $m_{11}^2 + m_{21}^2$, this square root is this value and then using this three, this one and the, so this three you are finding out m_{11} and m_{21} . So, from these two you are getting the relation between m_{11} and m_{21} that is less than you are getting.

Now, using this one, this normalization you are able to uniquely estimate the value of m_{11} and m_{21} . This is very simple one is, just you know are know1 thing you write down in terms of relation $m_{11} =$ in terms of m_{21} from the first equation and from the second equation you will get the similar thing. So, you need adage in financial number of solution to unique solution, because of this normalization. So, now, m_{11} m_{21} is known. So, with reference to λ_1 it is known. Now reference to λ_2 , second Eigen value, again find out the Eigen that m_{11} and m_{21} .

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Example: Second-order RSM (Contd.)

For $\lambda_1 = -1.4141$, $m_{11} = -0.9571$ and $m_{12} = 0.2898$

$$M = \begin{bmatrix} 0.2898 & -0.9571 \\ 0.9571 & 0.2898 \end{bmatrix} \quad (\because M = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix})$$

Relationship between x and w is:

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 0.2898 & 0.9571 \\ -0.9574 & 0.2898 \end{bmatrix} \begin{bmatrix} x_1 - 0.389 \\ x_2 - 0.306 \end{bmatrix}$$

↓

$$\begin{aligned} w_1 &= 0.2897(x_1 - 0.389) + 0.9571(x_2 - 0.306) \\ w_2 &= -0.9574(x_1 - 0.389) + 0.2888(x_2 - 0.306) \end{aligned}$$

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So, then you will ultimately found out the m m is 0 point this, this value you see m 11 28989 0.9571. So, 2898 0.9571 and this is from coming from the λ 2. Now w_1 w_2 equal to M transpose x minus x s , this you are getting and putting this you are getting this equation ok

So, put in this you are getting w_1 and w_2 . So, fine if we have w_1 value and w_2 value, you will get x_1 and x_2 . Once you get x_1 and x_2 you can convert to the original variable values and then you experiment there ok. So, this is what is the analysis part.

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References

- Design and Analysis of Experiments by Douglas Montgomery, Wiley, 8th Edition, 2014

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So, response surface methodology, I just conclude that. We have given you the approach, the purpose then we have shown you that to that is method of steepest methods of method of steepest ascent or descent, then first order model regression model, then second order regression model. How to compute all those things we have discussed their response surface designs then we have so now that way.

Then how to analyze the second order response surface and then when you are not in a position to operate the process in the point of maximum minimum or the stationary point, how to go to the next point of operation without incurring much losses. We have given you two kinds of analysis; contour plot base analysis and canonical analysis. So, all those are very very important and I hope that you will be able to answer the questions. So, that will be posted in the exam. And we will show you some of the Minitab based our computation in next few lectures.

Thank you very much.