Analysis of Variance and Design of Experiments-II

MODULE VIII

LECTURE - 35

RESPONSE SURFACE DESIGNS

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Analysis of a second-order response surface

When the experimenter is away from optimum, a lower order model is chosen to start with.

When the experimenter is relatively close to the optimum, then a model that incorporates curvature is usually required to approximate the response. In most cases, the second-order model is found to be suitable as

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

Now we discuss how to use this fitted model to find the optimum set of operating conditions for the x's and to characterize the nature of the response surface.

Location of the stationary point

Suppose we wish to find the levels of $x_1, x_2, \ldots, x_k$ that optimize the predicted response. This point, if it exists, will be the set of $x_1, x_2, \ldots, x_k$ for which the partial derivatives $\frac{\partial \hat{y}}{dx_1} = \frac{\partial \hat{y}}{\partial x_2} = \ldots = \frac{\partial \hat{y}}{\partial x_k} = 0.$

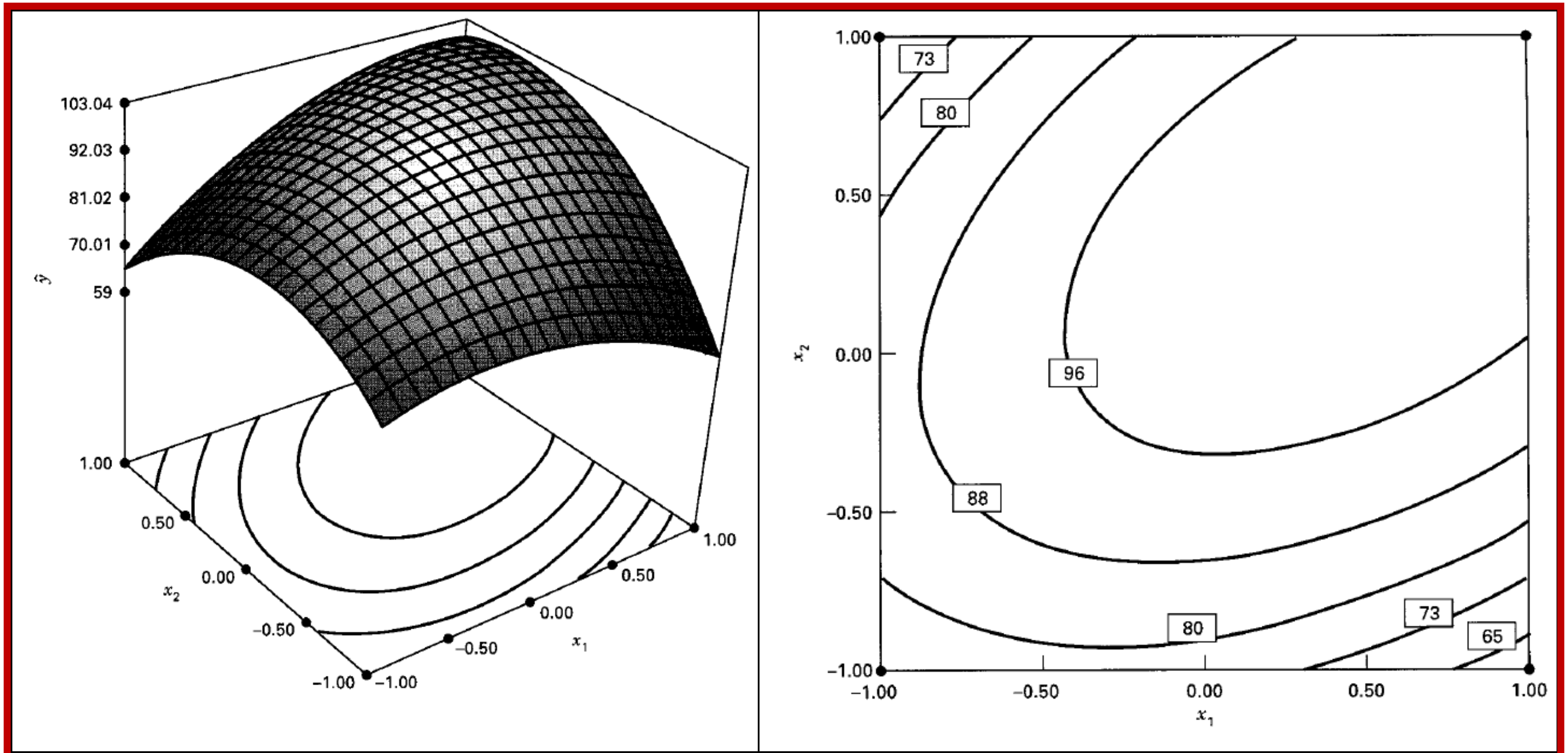
This point, say $x_{1,s}, x_{2,s}, \ldots, x_{k,s}$, is called the **stationary point**. The stationary point could represent

(1) a point of maximum response,

(2) a point of minimum response, or

(3) a saddle point.

These three possibilities are shown in the following figures:



Response surface and contour plot illustrating with a maximum

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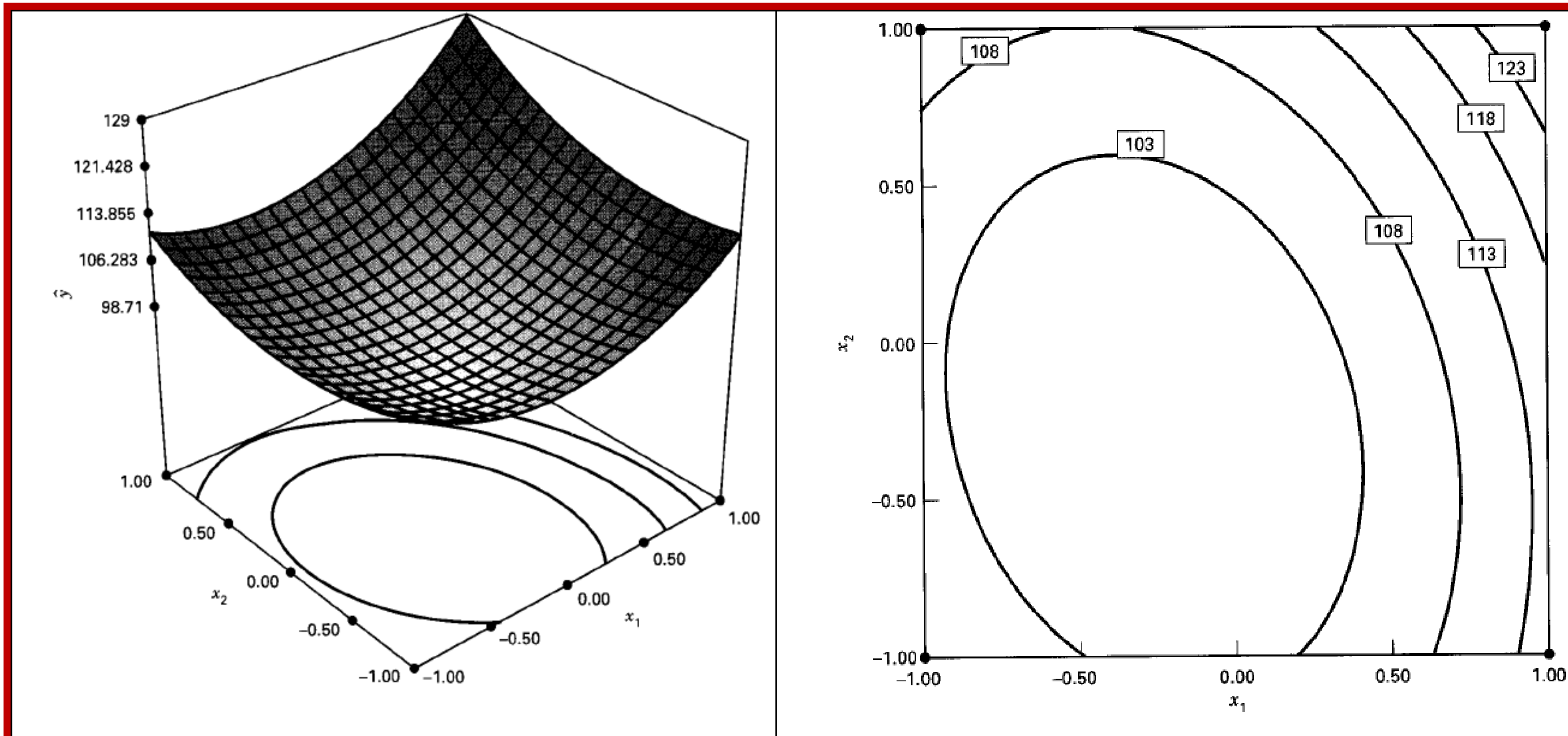

Response surface and contour plot illustrating with a minimum

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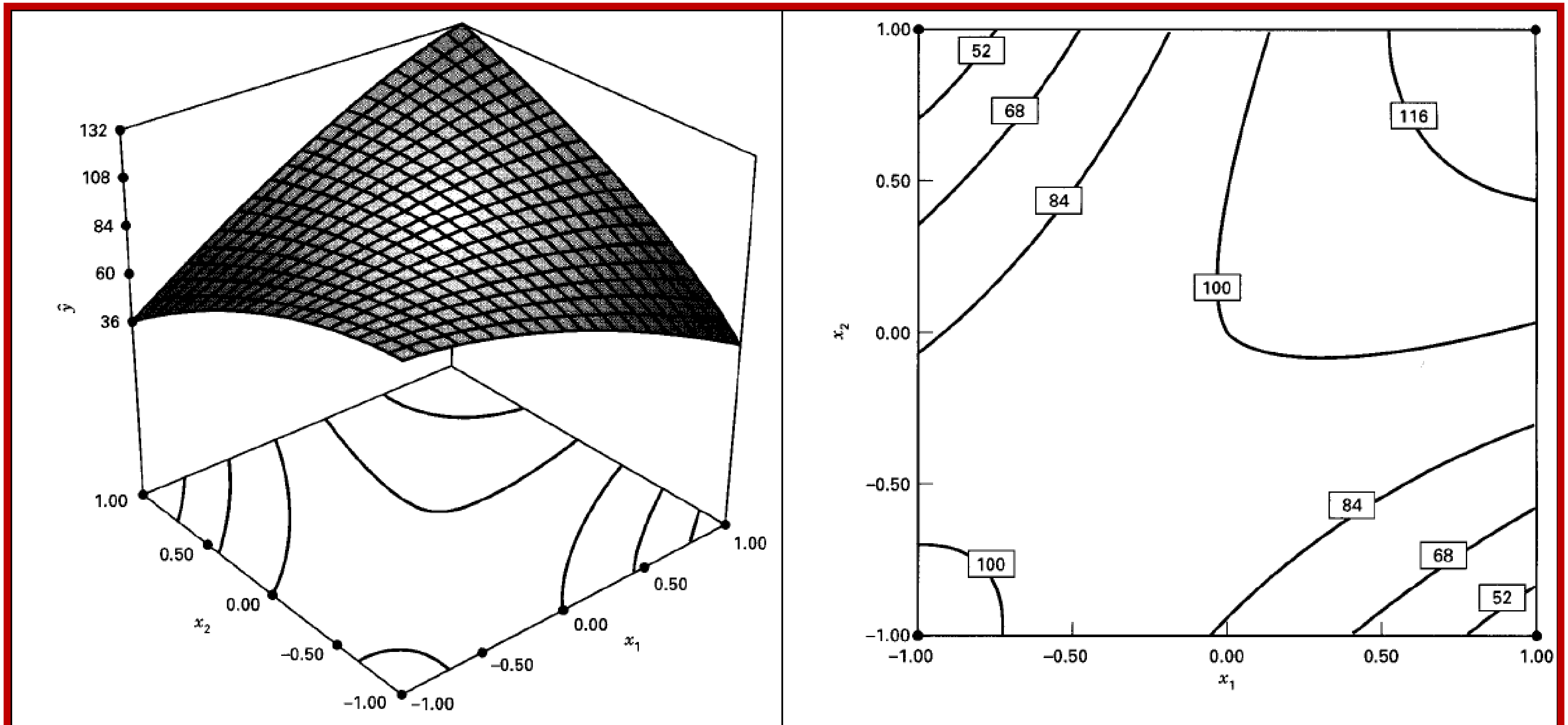

Response surface and contour plot illustrating a saddle point (or minimax)

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Contour plots are very important in the study of the response surface. Contours are generated with the help of computer software. Such contours help the experimenter in characterizing the shape of surface. This also helps is locating the optimum with reasonably lower variability.

We may obtain a general mathematical solution for the location of the stationary point. The second-order model can be expressed in matrix notations as

$$\hat{y} = \hat{\beta}_0 + x'b + x'Bx$$

where

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix}, \quad b = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} \hat{\beta}_{11}, & \hat{\beta}_{12}/2, & \ldots, & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22}, & \ldots, & \hat{\beta}_{2k}/2 \\ & & \ddots & \vdots \\ & & & \hat{\beta}_{kk} \end{bmatrix}$$

where *b* is a (*k* x 1) vector of the first-order regression coefficients and *B* is a (*k x k*) symmetric matrix whose main diagonal elements are the **pure** quadratic coefficients $(\hat{\beta}_{ii})$ and whose off-diagonal elements are one-half the **mixed** quadratic coefficients $(\hat{\beta}_{ij}, i \neq j)$. The stationary points obtained by solving $d\hat{y}/dx = 0$ as

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

which gives the stationary point as $x_s = -\frac{1}{2}B^{-1}b$

The predicted response at the stationary point is found by substituting x_s into $\hat{y} = \hat{\beta}_0 + x'b + x'Bx$ as

$$\hat{y}_s = \hat{\beta}_0 + \frac{1}{2}x_s'b.$$

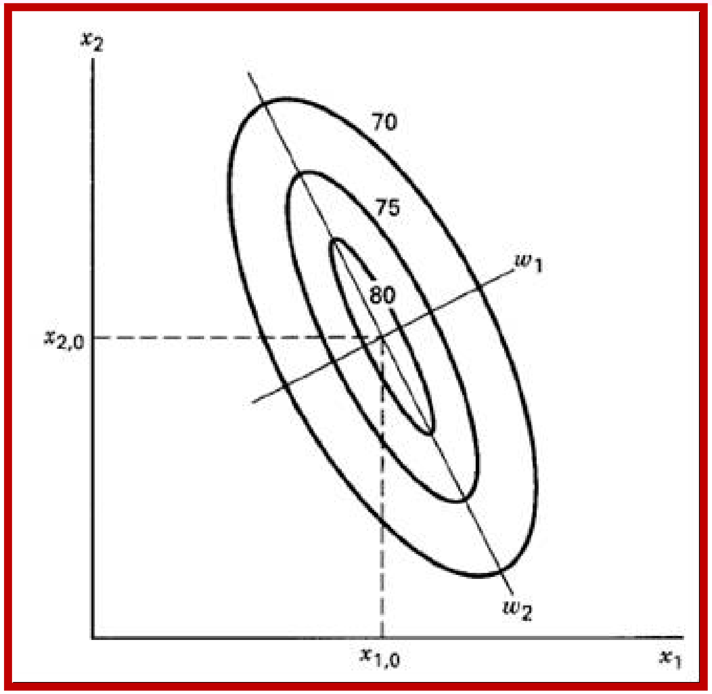
Characterizing the response surface

Once the stationary point is found then the response surface is characterized in the immediate vicinity of this point. The meaning of **characterize** is to determine whether the stationary point is a point of maximum or minimum response or a saddle point. The relative sensitivity of the response to the variables $x_1, x_2, .., x_k$ is also studied.

The most straightforward way to do this is to examine a contour plot of the fitted model. It is easier to study the contour plot if there are only two or three process variables (the *x's*), When there are relatively few variables, then the **canonical analysis** can be useful.

It is helpful first to transform the model into a new coordinate system with the origin at the stationary point x_5 and then to rotate the axes of this system until they are parallel to the principal axes of the fitted response surface. This transformation is illustrated in the following figure:

Canonical form of the second order model



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This results in the following fitted model

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

where the w_i's are the transformed independent variables and the λ_i's are constants. This equation is called the **canonical form of the model** and λ_i's are the **eigenvalues or characteristic roots of the matrix *B*.**

The nature of the response surface can be determined from the stationary point and the **signs and magnitudes** of the λ_i's. First suppose that the stationary point is within the region of exploration for fitting the second-order model.

If all $\lambda_i > 0 \Rightarrow x_s$ is a point of minimum response;

If all $\lambda_i < 0 \Rightarrow x_s$ is a point of maximum response; and

If λ_i's have different signs $\Rightarrow x_s$ is a saddle point.

Furthermore, the surface is steepest in the w_i direction for which λ_i is the greatest.

Experimental designs for fitting response surfaces

Fitting and analyzing response surfaces is greatly facilitated by the proper choice of an experimental design.

While selecting a response surface design, some of the features of a desirable design are as follows:

1. It provides a reasonable distribution of data points throughout the region of interest.
2. The model adequacy and the lack of fit can be checked.
3. It allows the experiments to be performed in blocks.
4. It permits to build the higher order designs sequentially.
5. It gives an internal estimate of error.
6. It yields the precise estimates of the model coefficients.
7. It provides a good profile of the prediction variance throughout the experimental region.
8. It shows reasonable robustness against outliers or missing values.
9. It does not require a large number of runs.
10. It does not require too many levels of the independent variables.
11. It ensures simplicity of calculation of the model parameters.

All these features may not always be meeting in a design, so judgment based on experience must often be applied in design selection