Analysis of Variance and Design of Experiments-II

MODULE VIII

LECTURE - 36

RESPONSE SURFACE DESIGNS

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Design for fitting the first-order model

Consider the following first-order model in *k* variables for fitting

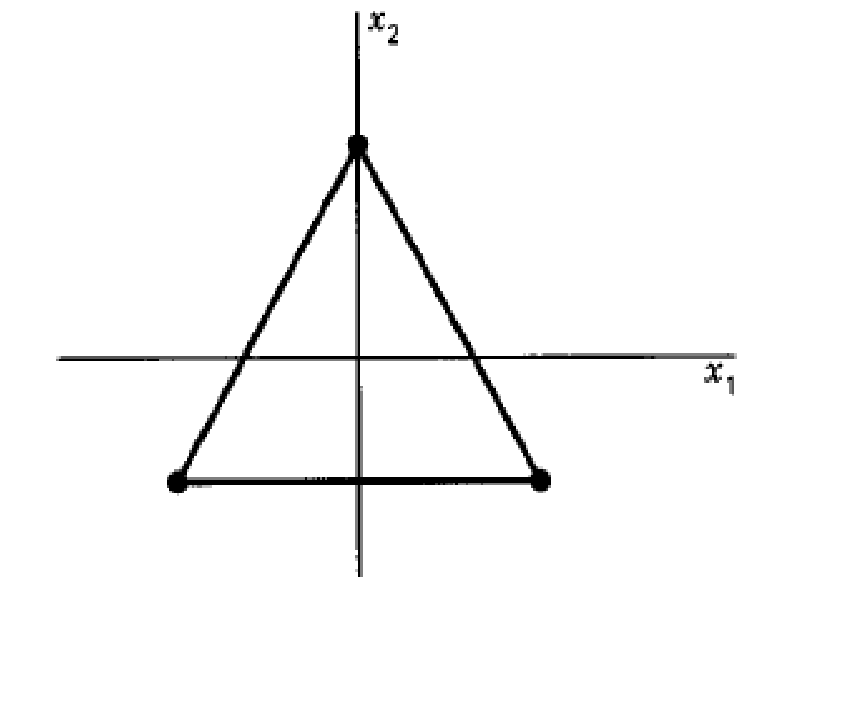
$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \varepsilon$$

There is a unique class of designs that minimize the variance of the regression coefficients $\hat{\beta}_i$'s. These are the **orthogonal first–order designs**. A first-order design is orthogonal if the off-diagonal elements of the $(X'X)$ matrix are all zero. This implies that the cross-products of the columns of the *X* matrix sum to zero.

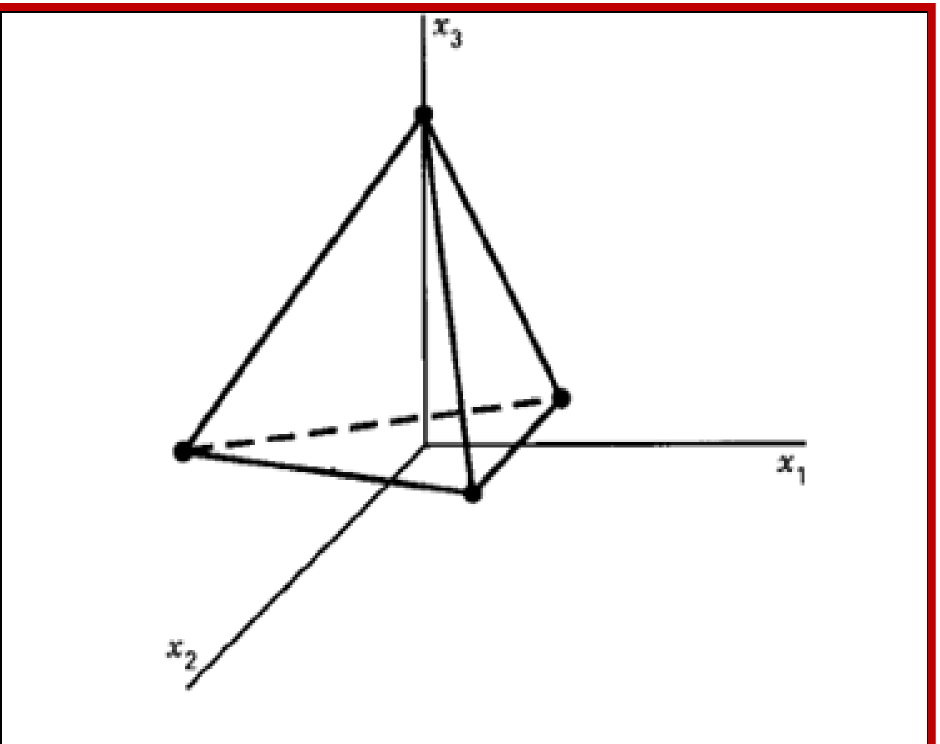
The 2^k factorial and fractions of the 2^k series in which main effects are not aliased with each other belongs to the class of orthogonal first-order designs. Assume that the low and high level of the *k* factors are coded as ± 1 levels to use is such designs.

The 2^k design cannot provide an estimate of the experimental error unless some runs are replicated. A method of including replication in the 2^k design is to augment the design with several observations at the center which is the point $x_i = 0, i = 1, 2, ..., k.$ The estimates of $\hat{\beta}_i$'s, $i \geq 1$ are not affected by adding the center points to the 2^k design. Only estimate of β_0 changes as it becomes the average of all the observations. The addition of center points does not alter the orthogonally property of the design.

Another orthogonal first-order design is the **simplex.** The simplex is a regularly sides figure with k + 1 vertices in k dimensions. Thus, for k = 2 the simplex design is an equilateral triangle and for k = 3 it is a regular tetrahedron. Simplex designs in two and three dimensions are shown in the following figure:



The simplex design for k = 2 variables



The simplex design for k = 3 variables

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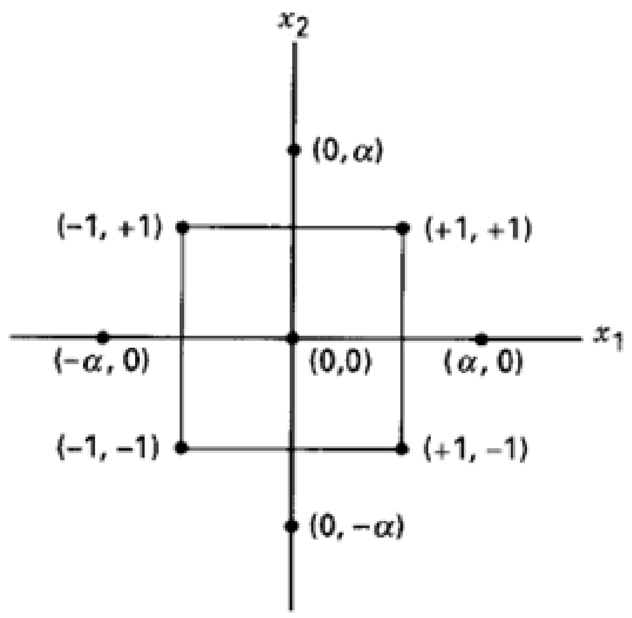
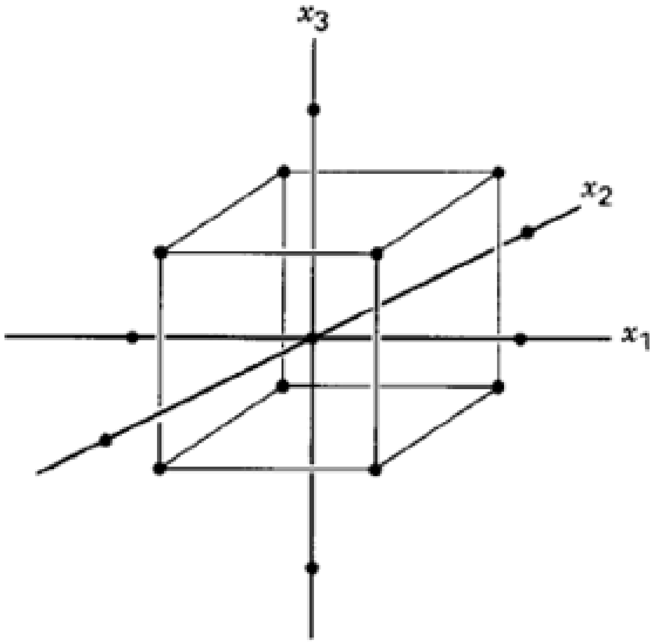
Designs for fitting the second-order model

The **central composite design** or **CCD** are used for fitting a second-order model. The CCD consists of a 2^k factorial with n_F runs, $2k$ axial or star runs , and n_c center runs. Following figure shows the CCD for $k = 2$ and $k = 3$ factors.

	
The central composite design for $k = 2$ variables	The central composite design for $k = 3$ variables

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The CCD is developed through **sequential experimentation**. Suppose a 2^k is used to fit a first-order model and suppose this model exhibits lack of fit. Then axial runs is added to allow the quadratic terms to be incorporated into the model. The CCD is a very efficient design for fitting the second-order model. There are two parameters in the design that must be specified:

- the distance α of the axial runs from the design center and
- the number of center points n_c.

We now discuss the choice of these two parameters.

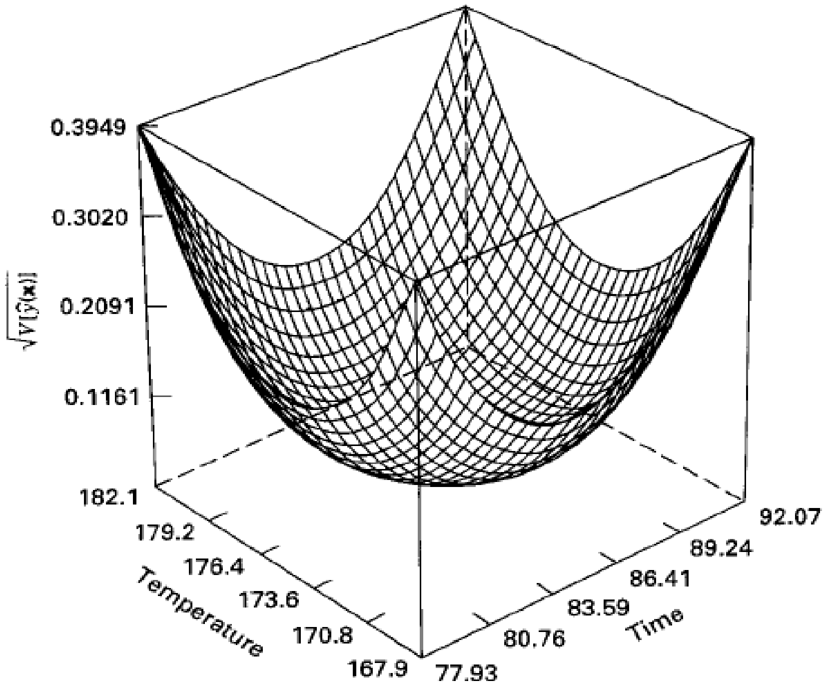
Readability

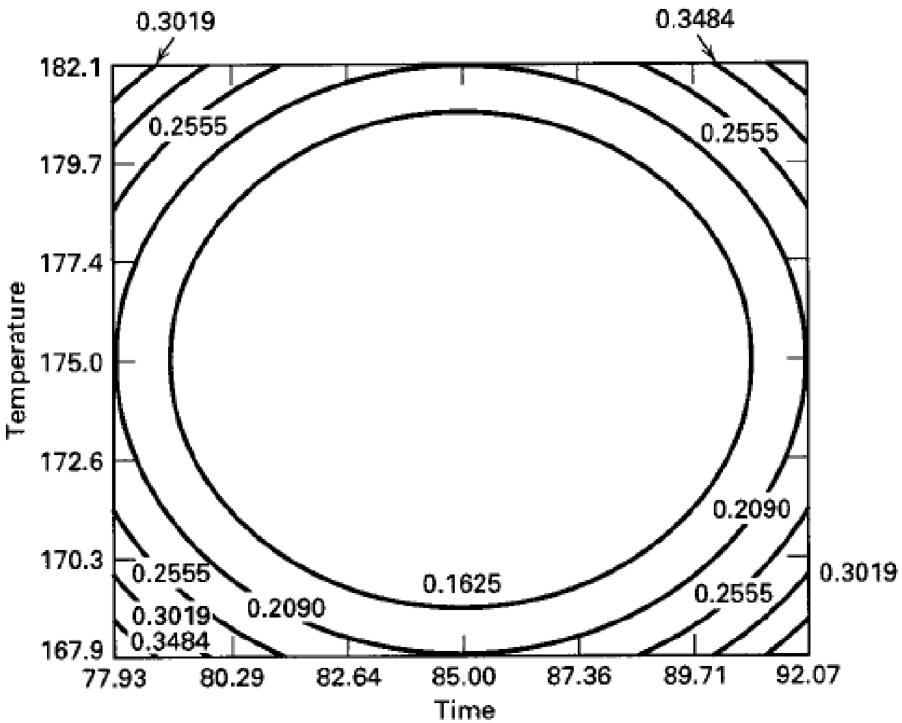
It is important for the second-order model to provide good predictions throughout the region of interest. One way to define "good" is to have the model which is a reasonably consistent and has stable variance of the predicted response at points of interest. The variance of the predicted response at some point *x* is

$$Var\left[\hat{y}(x)\right] = \sigma^2 x'(X'X)^{-1}x.$$

It is suggested that a second-order response surface design should be **rotatable**. This means that the $Var\left[\hat{y}(x)\right]$ is the same at all points *x* that are at the same distance from the design center. That is, the variance of predicted response is constant on spheres.

Following figure shows contours of constant $\sqrt{Var\left[\hat{y}(x)\right]}$ for the second-order model fit using the CCD.





Contours of constant standard deviation of predicted response for the rotatable CCD

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Notice that the contours of constant standard deviation of predicted response are concentric circles. A design with this property will leave the variance of $\hat{y}$ unchanged when the design is rotated about the center (0, 0,…,0). Hence it is termed as **rotatable design.**

Rotatability is an important criterion for the selection of a response surface design. The aim of RSM is optimization and the location of the optimum is unknown prior to running the experiment, so it makes sense to use a design that provides equal precision of estimation in all the directions. In fact, any first–order orthogonal design is rotatable.

A central composite design is made rotatable by the choice of α. The value of α for rotatability depends on the number of points in the factorial portion of the design. The choice $\alpha = (n_F)^{1/4}$ yields a rotatable central composite design where n_F is the number of points used in the factorial portion of the design.

The spherical CCD

Rotatability is a spherical property. It is an important design criterion when the region of interest is a sphere. It is not important to have the exact rotatability to have a good design. The best choice of α for a spherical region of interest from a prediction variance view point for the CCD is to set $\alpha = \sqrt{k}.$ This design called a **spherical CCD.** This puts all the factorial and axial design points on the surface of a sphere of radius $\sqrt{k}.$

Center runs in the CCD

The choice of α in the CCD is dictated primarily by the region of interest. When this region is a sphere, the design must include center runs to provide reasonably stable variance of predicted response. Generally, three to five center runs are recommended.

Blocking in response surface designs

When using the response surface designs, it is often necessary to consider blocking to eliminate nuisance variables. Such problem may occur when a higher order, say second-order design is assembled sequentially from lower order, say. Such necessity arises due to various reasons. For example, considerable time may elapse between the running of the first-order design and the running of the supplemental experiments which are required to build up a second-order design, and during this time, the test conditions may change which makes necessary to use blocking.

A response surface design is said to be **block orthogonally** if it is divided into blocks such that block effects do not affect the parameter estimates of the response surface model. If a 2^k or 2^{k-p} design is used as a first-order response surface design, the center points in these designs should be allocated among the blocks.

For a second-order design to block orthogonally, two conditions must be satisfied. If there are n_b observations in the b^{th} block, then these conditions are

1. Each block must be a first-order orthogonal design; that is, $\sum_{u=1}^{n_b} x_{iu} x_{ju} = 0 \quad i \neq j = 0, 1, \ldots, k$ for all b

   where x_{iu} and x_{ju} are the levels of i^{th} and j^{th} variables in the u^{th} run of the experiment with $x_{0u} = 1$ for all u.

2. The fraction of the total sum of squares for each variable contributed by every block must be equal to the fraction of the total observations that occur in the block; that is,

$$\frac{\sum_{u=1}^{n_b} x_{iu}^2}{\sum_{u=1}^{N} x_{iu}^2} = \frac{n_b}{N} \qquad i = 1, 2, \ldots, k \text{ for all } b$$

   where N is the number of runs in the design.