In order to get the relation between the response and the factor levels the treatment combinations have to be suitable chosen. The treatment combinations of the ordinary full factorial need not be the best for fitting the relation. It is therefore, necessary to search for the suitable set of treatment combinations by using which a stipulated relation can be fitted. Such a set of treatment combination is called a *response surface design*. Actually the factor-esponse relationship is called response surface. These surface can be linear, second degree and third degree polynomials, and so on. We shall discuss here only the first and second degree surfaces, construction of designs suitable for fitting them and method of interpretation of the data.

7.7.5 Rotatable Designs

A second degree response surface design will be called a second order rotatable design if in this design $c = 3$ and all the other conditions enumerated earlier hold. Formally a second order rotatable design can be defined as below.

A design is said to be second order rotatable design if a second degree surface of the form

$$y = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_{ii} x_i^2 + \ldots + b_{ij} x_i x_j + \ldots$$

of the response as obtained from the design points on the variates $x_i (i=1, 2, \ldots, v)$ with some suitable origin and scale can be so fitted that the variance of the estimate of the response from any treatment combination is a function of the sums of squares of the levels of the factors in that treatment combination (see Box and Hunter, 1957).

7.7.8 Construction

A full factorial of the series 3^n or a suitable fraction of the same, in which no interaction with less than 5 factors is confounded, will always provide a second order response surface design when the origin is shifted to the middle of the range of each factor and then a suitable scale change is made. These designs are not rotatable but will have a value of 1.5 for c.

Construction of Second Order Rotatable Designs

There are several methods of construction of such designs. Some of these methods have been described below.

Method I

Let there be v factors. Each of these factors is taken at a certain number of levels. Some of these levels are denoted by one or more unknowns like a, b, etc. Thus, we shall have treatment combinations like $aao\ldots b$. We shall not take all such combinations but several of them as the situation demands. Next, another design 2^v is taken. In this design each of the factors is taken at levels + 1 and – 1.

Each of the combinations of the unknown levels, a, *b*, *o*, etc. which have been taken for constructing the design is then associated with each of the combinations of the 2^v design. The rule of association is that the corresponding entries in the two combinations, *viz*, one involving the unknowns and the other coming from the 2^v factorial are multiplied and the products are written in the same order. This last combination obtained from the products is a design point. Thus out of each combination involving the unknowns without sign we shall get design points after association. For example, if we have the combination *aab* involving the unknowns *a* and *b*, we have first to take a 2^3 factorial written by the levels + 1 and – 1 for each factor. This factorial is

–1	–1	–1
–1	–1	1
–1	1	–1
–1	1	1
1	–1	–1
1	–1	1
1	1	–1
1	1	1

Now by associating the combination *aab* with each of the above combinations of the 2^3 factorial we get

$-a$	$-a$	$-b$
$-a$	$-a$	b
$-a$	a	$-b$
$-a$	a	b
a	$-a$	$-b$
a	$-a$	b
a	a	$-b$
a	a	b

These eight combinations are the design points.

If we take the combination *oab* instead of *aab*, we find that by the above method of association we get the following design points.

o	$-a$	$-b$
o	$-a$	b
o	a	$-b$
o	a	b
o	$-a$	$-b$
o	$-a$	b
o	a	$-b$
o	a	b

It is seen that these eight points are not distinct but the last four are repetitions of the first four. This has happened because by associating + 1 or –1 to zero we do not get different levels. Thus to get distinct design points which is normally required, we have to associate a combination of the unknowns with the 2^P factorial in place of the 2^v factorial where p is the number of non–zero unknowns in the combination taken. Thus with the combination oab we have to associate a 2^2 and not a 2^3 factorial.

This way of obtaining design points by associating with a 2^p factorial ensures that the sum of products of powers of x_i's in which at least one x_t is an odd power, is zero. But this does not ensure that the other conditions are satisfied.

A further criterion for choosing p in the $2p$ factorial when p is greater than 4, is that for satisfying the above condition, we may also take a fraction of $2p$ for which the defining contrasts must not involve any interaction with less than five factors as no sum of products of the x_i's is of more than the fourth degree. Now for satisfying the other conditions like $\sum x_i^2 = N\lambda_2$ or $\sum x_i^4 = 3N\lambda_4$ or $\sum x_i^2 x_j^2 = N\lambda_4$ we have to take some more combinations of the unknowns, in such a manner that each factor gets a chance to have the same set of levels.

For example, when we take the combination oab all the three factors are at different levels. In order to ensure that each factor occurs at the same set of levels we have to choose the following combinations, obtained by cyclically changing the above levels of the three factors :

o	a	b
a	b	o
b	o	a

Next, by associating each of the above combinations with the 2^2 factorial we get the following design points:

o	a	b
o	a	$-b$
o	$-$ a	b
o	$-$ a	$-b$
a	b	o
$-a$	$-b$	o
$-a$	b	o
a	$-b$	o
b	o	a
b	o	$-a$
$-b$	o	a
$-b$	o	$-a$

It is easily seen that the above points satisfy each of the conditions $\Sigma x_i^2 =$ constant, $\Sigma x_i^4 =$ constant and $\Sigma x_i^2 x_j^2 =$ constant. For the above combinations we find

$$\sum x_i^2 = 4(a^2 + b^2), \sum x_i^4 = 4(a^4 + b^4) \text{ and} \sum x_i^2 x_j^2 = 4a^2 b^2.$$

In order to satisfy the condition that $\sum x_i^4 = 3\sum x_i^2 x_j^2$ we require that

$$4(a^4 + b^2) = 3 \times 4a^2 b^2$$

or

$$x^2 - 3x + 1 = 0 \text{ where } x = \frac{b^2}{a^2}.$$

This condition thus gives an equation involving two unknowns and one of the unknowns can therefore be chosen so as to satisfy the above relation. The other unknown can be fixed arbitrarily.

It will be seen that the condition $\lambda_4/\lambda^2_2 > v/(v+2)$ which follows from $\lambda_4/\lambda^2_2 > v/(v+c-1)$ for the general response surface designs, is not satisfied in the above design. As a matter of fact if all the points in a design are equidistant from the origin as in this design, then the above condition is not satisfied. As a remedy, a central point of the form (0, 0, 0) is taken and the above condition then holds. Addition of such central points does not disturb any other requirement.

Thus, by taking say "a" as 1 arbitrarily, then obtaining b from the above equation and finally taking a central point we get a second order rotatable design in 13 points with each factor occurring at the five levels

$$-1.62, -1, 0, 1, 1.62$$

In order to transform the above levels to actual levels first the range of the levels of each factor is fixed. Let such ranges for a factor be R_0 and R_M. Thus $-b$ corresponds to the minimum R_0 and b corresponds to R_M. As the coded doses are linear transforms of the real doses, we assume that the coded dose, say, y is connected with the real dose, say x, through the relation $y = \alpha + \beta x$. Now two points on the line, *viz.* $(R_0, -b)$ and (R_M, b) are known. Hence substituting these two points in the equation α and β can be obtained. Once the relation $y = \alpha + \beta x$ is thus established the other real doses corresponding to $-a$, o and a can easily be obtained from it.

Method II: Central Composite Designs

The central composite designs are obtained by taking the following combinations of the unknowns

$$a, a, a, \ldots, a$$

$$b, 0, 0, \ldots, o,$$

$$o, b, o, \ldots, o,$$

$$o, o, b, \ldots, o$$

$$\ldots\ldots\ldots\ldots\ldots\ldots$$

$$o, o, o, \ldots, b$$

Next a suitable fraction of the 2^V factorials is associated with the first combination. From each of the other v combinations like $(b\ o \ldots o)$, we get two combinations, *viz.*, $(b\ o\ o \ldots o)$ and $(-b\ o \ldots o)$. When $v = 4$ we have also to take a central point. The values of a and b can be obtained by using the condition

$$\sum x_i^2 = 3\sum x_i^2 x_j^2$$

and fixing one of them arbitrarily.

For example, when $v = 5$, we have the combinations

$$\begin{array}{ccccc} a & a & a & a & a \\ b & o & o & o & o \\ o & b & o & o & o \\ o & o & b & o & o \\ o & o & o & b & o \\ o & o & o & o & b \end{array}$$

We shall associate $a(1/2)(2^5)$ fraction with the first combination. The $\frac{1}{2}$ fraction is obtained by confounding the 5-factor interaction in 2^5. This design will have thus $16 + 10 = 26$ design points

Then $$\sum x_i^4 = 16a^4 + 2b^4$$

and $$\sum x_j^2 x_i^i = 16a^4$$

Hence we have the equation

$$16a^4 + 2b^4 = 3 \times 16\, a^4$$

giving $$b^4 = 16\, a^4$$

i.e. $$b = 2a$$

Taking, $a = 1$, we get $b = 2$ and hence the five levels are $-2, -1, 0, 1$ and 2.

Method III

Use of balanced incomplete block designs for construction of second order rotatable designs (Das and Narasimhan, 1962).

First the incidence matrix of a balanced incomplete block design is taken. The element 1 in it is replaced by an unknown a. From the rows of this matrix involving 0 and the unknown a, we shall get b combinations. Each of these combinations is then associated with 2^k factorial or a suitable fraction, say 2^p, of it. We shall thus get $\sum x_i^2 = r\, 2p\, a^4$ (taking $k = p$ when a fractional factorial is used) and $\sum x_i^2 x_j^2 = \lambda 2_p$ a^4. It is now required that $\Sigma\, x_i^2 = 3\,\Sigma\, x_i^2 x_j^2$. That is, $r2pa^4 = 3\lambda 2pa^4$ or $r = 3\lambda$. It may happen that such a BIB design actually exists. In that case no further combinations need be taken excepting a central point, which is necessary as all such points are at a distance equal to ka^2 from the origin.

For example in the BIB design $v = 7$, $b = 7$, $r = k = 3$, $\lambda = 1$, we have $r = 3\lambda$.

Hence, from the incidence matrix of this design we can get the following design. The incidence matrix is given by

1	1	0	1	0	0	0
0	1	1	0	1	0	0
0	0	1	1	0	1	0
0	0	0	1	1	0	1
1	0	0	0	1	1	0
0	1	0	0	0	1	1
1	0	1	0	0	0	1

Replacing 1 by a we get the following seven combinations of the unknown level a;

a	a	0	a	0	0	0
0	a	a	0	a	0	0
.	.	.	.	.	.	.
a	0	a	0	0	0	a

From the first combination we get the following points by associating with a 2^3 factorial:

$$\begin{array}{ccccccc}
a & a & 0 & a & 0 & 0 & 0 \\
a & a & 0 & -a & 0 & 0 & 0 \\
a & -a & 0 & a & 0 & 0 & 0 \\
a & -a & 0 & -a & 0 & 0 & 0 \\
-a & a & 0 & a & 0 & 0 & 0 \\
-a & a & 0 & -a & 0 & 0 & 0 \\
-a & -a & 0 & a & 0 & 0 & 0 \\
-a & -a & 0 & -a & 0 & 0 & 0
\end{array}$$

Associating the 2^3 factorial with the other combinations as well, we shall get in all 56 design points. These points along with the central point (0 0 0 0 0 0 0) give a second order rotatable design in 57 points with each factor at three levels $-a$, 0, a. In this design, we have:

$$\sum x_i^4 = 24a^4$$

$$\sum x_i^2 x_j^2 = 8a^4$$

Hence the condition $\sum x_i^4 = 3\sum x_i^2 x_j^2$ is automatically satisfied. The unknown "a" can now be fixed arbitrarily.

If however, the relation $r = 3\lambda$ does not hold in a BIB design, we have to take further combinations of another unknown b as below.

If $r < 3\lambda$, we have to take the combinations

$$\begin{array}{ccccc}
b & 0 & 0 & \ldots & 0 \\
0 & b & 0 & \ldots & 0 \\
0 & 0 & b & \ldots & 0 \\
. & . & . & . & . \\
0 & 0 & 0 & \ldots & b
\end{array}$$

For example in the design $v = b = 3$, $r = k = 2$, $\lambda = 1$ we have $r < 3\lambda$. The incidence matrix of this design is given by

$$\begin{array}{ccc}
1 & 1 & 0 \\
0 & 1 & 1 \\
1 & 0 & 1
\end{array}$$

Hence unknowns combinations are

$$\begin{array}{ccc}
a & a & 0 \\
0 & a & a \\
a & 0 & a
\end{array}$$

These combinations with the further three combinations

$$\begin{matrix} b & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & b \end{matrix}$$

will give a design in three factors with 18 points.

The values of the unknowns have to be fixed in this case by using the relation $\sum x_i^4 = 3\sum x_i^2 x_j^2$.

If again $r > 3\lambda$, the combination $(b, b, \ldots, b)$ has to be taken along with the combinations obtained from the incidence matrix of the BIB design.

For example, in the design $v = 5$, $b = 10$, $r = 4$, $k = 2$, $\lambda = 1$ we nave $r > 3\lambda$.

Hence along with the 10 combinations obtained from the BIB design, we have to take the further combination

$$(b\ b\ b\ b\ b)$$

From the last combination we shall get 16 design points as we have to use a half fraction of 2^5 for association.

The total number of points in this design will thus be

$$(4 \times 10) + 16 = 56$$

Here, again the restriction $\sum x_i^4 = 3\sum x_i^2 x_j^2$ has to be used for determining one of the unknown levels.

When we have obtained a design in v factors by any of the above methods, we can always obtain a design in $v - s$ factors by omitting any s columns of the design matrix.

In addition to the above methods there are several other convenient methods for construction of such designs. For details the reader is referred to the references mentioned at the end of this chapter.