A TYPE OF CENTRAL COMPOSITE RESPONSE SURFACE DESIGNS

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INTRODUCTION

For the exploration of response surfaces Box and Hunter (1957)[1] introduced rotatable designs. Though these designs have been applied extensively for the industrial and engineering experiments, their application for agricultural experiments seems to be limited. R.M. De Bann (1959)[4] discussed first 3-factor response surface designs. W.M. Walker, J. Pesek and E.O. Heady (1963)[5] applied a central composite design in three factors for studying the effects of Nitrogen, Phosphorus and Potassium fertilizers on the economics of producing blue grass forage. The design adopted by them was a second order central composite rotatable design in all respects excepting that they look five equi-spaced doses for each of the factors instead of those required by the corresponding rotatable design. As a result, the design became one corresponding to the rotatable design in which all the relations excepting $\Sigma x_i^4 = 3\Sigma x_i^2 x_j^2$ were satisfied. Equispaced doses for each of the factors are normally preferred by the experimenters. This requirement is normally not satisfied in most of the rotatable designs, where the factors are at 5 or more levels. The purpose of the present paper is to investigate the consequence of taking a central composite rotatable design first, and making the doses of each factor equi-spaced. We have called these designs central composite non-rotatable designs or in short central composite designs and discussed their construction below.

CONSTRUCTION

Taking x_i as the variate denoting the levels of the i^{th} of the v factors $(i = 1, 2, \dots v)$, in a central composite rotatable design, the relations in rotatable designs can be divided into two main groups as below : [Das and Narasimhan (1962)[3] and Das (1963)[2]].

Group (a) (i) $\Sigma x_i = 0 \quad \Sigma x_i x_j = 0$ ... etc.

(ii) $\Sigma x_i^2 = \text{const.}$

$\Sigma x_i^4 = \text{const.}$

$\Sigma x_i^2 x_j^2 = \text{const.}$

Group (*b*) $\Sigma x_i^4 = 3\Sigma x_i^2 x_j^2$.

The above summations are over the design points.

The group (*a*) relations simplify the solution of the normal equations for estimating the parameters in the surface, while the relation in group (*b*) makes the design rotatable, so as to make the variance at a particular point a function of the distance of the point from the origin. Due to this restriction in group (*b*) the doses of any particular function cannot be spaced arbitrarily. This puts a limitation on the design as the doses are often fractional or even irrational. We have, therefore, attempted to obtain a type of designs from the rotatable designs by waiving the condition of the rotatability and taking the levels equi-spaced. Thus the number and nature of the combinations in the design just defined and those in the rotatable design are the same, but the levels of the different factors in the two designs are different. For example, from the following central composite rotatable design in three factors we can obtain the following central composite design.

Rotatable central composite design in 3 factors written in level codes :—

				New Design	
—1·08	—1·08	—1·08	—1	—1	—1
—1·08	—1·08	1·08	—1	—1	1
—1·08	1·08	—1·08	—1	1	—1
—1·08	1·08	1·08	—1	1	1
1·08	—1·08	—1·08	1	—1	—1
1·08	—1·08	1·08	1	—1	1
1·08	1·08	—1·08	1	1	—1
1·08	1·08	1·08	1	1	1
1·82	0	0	2	0	0
—1·82	0	0	—2	0	0
0	1·82	0	0	2	0
0	—1·82	0	0	—2	0
0	0	1·82	0	0	2
0	0	—1·82	0	0	—2
0	0	0	0	0	0

The new design presented side by side is obtained by taking the levels as -2, -1, 0, 1, and 2 ; *i.e.*, by replacing the dose $-1·82$ by -2, $-1·08$ by -1, 0 by 0, 1·08 by 1 and 1·82 by 2, in the above rotatable design.

It will be seen that in the new design or in general for any such design obtained from a corresponding rotatable design all the relations in group (*a*) will be satisfied. As a matter of fact Σx_i^4 will generally be *c* times $\Sigma x_i^2 \; x_j^2$, where *c* is a constant whose value depends on the design and the number of factors. In rotatable design the value of *c* is 3.

Analysis of the Design

The analysis of the central composite designs obtainable from the central composite rotatable designs has been discussed. Let there be *v* factors. Let the number of design points obtainable from the set $(a, a, \ldots a)$ be *n* and therefrom the sets $(b, 0, \ldots 0)$ are $2v$. The relations for the rotatable design reduce to the following in the case of central composite designs obtained from the above central composite rotatable design.

$$\Sigma x_i^2 = n+8 = N\lambda_2$$
$$\Sigma x_i^4 = n+32$$
$$\Sigma x_i^2 x_j^2 = n = N\lambda_4$$

where *N* is the total number of treatment combinations in the design. Sum of squares with at least one *x* with odd power is zero.

Taking the equation of the surface to be fitted through the above design as

$$\Upsilon = b_o + \Sigma b_i x_i + \Sigma b_{ii} \, x_i^2 + \sum_{i \neq j} b_{ij} \, x_i x_j$$

the solution of the normal equations for estimating the parameters of the surface through the method of least squares comes out as given below :

$$b_o = \frac{1}{N} \Sigma y - \frac{\lambda_2}{N} \left[\sum_i \frac{(\Sigma x_i^2 y) - v\lambda_2 \, \Sigma y}{\lambda_4 \, (c+v-1) - v\lambda_2^2} \right]$$

$$b_i = \frac{\Sigma \, x_i y}{N\lambda_2}$$

$$b_{ij} = \frac{\Sigma \, x_i x_j y}{N\lambda_4}$$

$$b_{ii} = \frac{1}{N\lambda_4(c-1)} \left[\Sigma x_i^2 y - \lambda_2 \, \Sigma y + (\lambda_2^2 - \lambda_4) \times \left\{ \sum_i \frac{(\Sigma x_i^2 y) - v\lambda_2 \, \Sigma y}{\lambda_4 \, (c+v-1) - v\lambda_2^2} \right\} \right].$$

The variances and covariances of the parameters are also shown below:

$$V(b_o)=\lambda_4\,(c+v-1)\,D\sigma^2$$

where

$$D=[N\,\{\lambda_4\,(c+v-1)-v\lambda_2^2\}\,]^{-1}.$$

$$\text{Cov}\,(b_o,\,b_{ii})=-\lambda_2 D\sigma^2$$

$$V\,(b_i)=\frac{1}{N\lambda_2}\,\sigma^2$$

$$V\,(b_{ii})=\frac{D}{\lambda_4\,(c-1)}\,[\lambda_4\,(c+v-2)-(v-1)\,\lambda_2^2]\,\sigma^2$$

$$V\,(b_{ij})=\frac{1}{N\lambda_4}\,\sigma^2$$

$$\text{Cov}\,(b_{ii},\,b_{jj})=\frac{D}{\lambda_4(c-1)}\,[\lambda_2^2-\lambda_4]\,\sigma^2$$

The covariances between any other pair *of* b's are zero.

The variance of a response $\hat{y}_o$ estimated through the surface at the point $(x_{10},\, x_{20},\, \ldots\, x_{vo})$ comes out as

$$V\,(\hat{y}_o)=V(b_o)+D^2\left[\frac{1}{N\lambda_2}-2\lambda_2 D\right]\sigma^2+d^4V\,(b_{ii})$$
$$+\frac{(c-3)}{(c-1)\,\lambda_4 N}\,\sigma^2\,\Sigma x_{io}^2\,x_{jo}^2$$

For the central composite designs the variance of an estimated response is not in general a function of the distance of the point from the origin.

As $N=n+2v+P$ where P denotes the number of central points, we can simplify the above variances etc. as shown below.

The variance of a response $\hat{y}_o$ estimated through the surface at the point $(x_{10},\, x_{20},\, \ldots\, x_{vo})$ comes out as

$$V\left(\hat{y}_o\right)=\frac{(nv+32)}{2n(v-4)^2+P(nv+32)}\,\sigma^2$$
$$+\left[\frac{2nv(v-8)+P(nv+32)-2(n^2+64)}{(n+8)\{2n(v-4)^2+P(nv+32)\}}\right]d^2\sigma^2$$
$$+\left[\frac{2nv(v-9)+16(3n+4)+P(nv-n+32)}{32\{2n(v-4)^2+P(nv+32)\}}\right]d^4\sigma^2$$
$$+\frac{16-n}{16n}\,\sigma^2\,\Sigma x_{io}^2\,x_{jo}^2.$$

The analysis of variances partition for such a design without replication is as follows :

Source	d.f.
Fitted constants	Total no. of constants -1
Lack of fit	Total no. of distinct combinations—no. of constants.
Error	$p-1$
Total	$N-1$.

COMPARISON OF THE NEAR ROTATABLE DESIGNS WITH THE CORRESPONDING ROTATABLE DESIGNS

For the purpose of comparison we shall take the number of design points in both the designs the same. The value of λ_2 will also be equalised for both the designs. As the value of λ_2 in the new design is $\frac{n+8}{N}$ we have first obtained the different variance function of the rotatable design in terms of λ_2, though such variances are usually worked out by taking $\lambda_2=1$.

The variance of an estimated response, $\hat{y}_o'$ at a distance 'd' from the origin estimated through the rotatable design comes out as shown below :

When $\lambda_2=\frac{n+8}{N}$

$$V\left(\hat{y}_o'\right)=V(b'_o)+\left(\frac{1}{N\lambda_2}-2\lambda_2 D\right)d^2\sigma^2+V(b'_{ii})d^4$$

$$=\frac{(v+2)}{[(v+2)(n+2v)-v(2+\sqrt{n})^2]}\sigma^2$$

$$+\frac{2(v+2)(v+2\sqrt{n}-2)}{(n+8)\{(n+2v)(v+2)-v(2+\sqrt{n})^2\}}d^2\sigma^2$$

$$+\frac{(2+\sqrt{n})[(v-1)(v-2\sqrt{n})+n+2]}{(n+8)^2[(n+2v)(v+2)-v(2+\sqrt{n})^2]}d^4\sigma^2$$

The variance of response at the same point estimated through the near rotatable design presented in the previous sections comes out as—

$$V\left(\hat{y}_o\right)=\frac{(nv+32)\sigma^2}{2n(v-4)^2}+\frac{2nv(v-8)-2(n^2+64)^2}{2n(n+8)(v-4)^2}d^2\sigma^2$$

$$+\frac{2nv(v-9)+16(3n+4)}{64n(v-4)^2}d^4\sigma^2$$

$$+\frac{16-n}{16n}\sigma^2\,\Sigma x_{io}^2\,x_{jo}^2$$

The first terms in each of the above two variance expressions is the variance of the response at the central point (0, 0, ... 0) estimated through the two designs. It can be shown that $V(b'_o)$ is always greater than $V(b_o)$ for all designs in which n, the number of design points from the set $(a, a, \ldots a)$ is the minimum possible. This shows that the near rotatable design provides more precise estimates.

AN ILLUSTRATIVE EXAMPLE

The following is the data from an experiment on blue grass yields reported by William M. Walker, John Pesek, and Earl O. Heady (1963). The following 15 combinations of nitrogen, phosphorus and potassium fertilizer were taken for the experiment.

	lb per acre		*yield*	*N*	*P*	*K*	*Yield*
N	*P*	*K*	*lb/acre*	X_1	X_2	X_3	*Y*
40	13	17	1780	−1	−1	−1	1780
40	13	50	2370	−1	−1	1	2370
40	39	17	1880	−1	1	−1	1880
40	39	50	2380	−1	1	1	2380
120	13	17	3140	1	−1	−1	3140
120	13	50	3540	1	−1	+1	3540
120	39	17	3530	1	1	−1	3530
120	39	50	3730	1	1	1	3730
80	26	33	3260	0	0	0	3260
0	26	33	1460	−2	0	0	1460
160	26	33	4240	2	0	0	4240
80	0	33	1970	0	−2	0	1970
80	52	33	2840	0	2	0	2840
80	26	0	3300	0	0	−2	3300
80	26	66	2830	0	0	2	2830

The doses of nitrogen were taken as 0 lb, 40 lbs, 80 lbs, 120 lbs and 160 lbs per acre. Similar nearly equispaced doses were used for the other two fertilizers.

To make the above design rotatable the doses for nitrogen shown be 0, 33, 80, 127, 160 in the above units. For the other two fertilizers the doses should be 0, 8, 20, 31 and 39 for phosphorus 0, 14, 33, 52, and 66 for potassium.

By changing the origins to 80, 26, 33, for N, P and K respectively we can write the data along with the transformed doses as shown side by side in the above table.

ANALYSIS

Sum of squares due to the fitted constants is the same as the sum of squares due to regression. This can be split into linear quadratic effects of the main effects and the linear interaction effects are as shown below:

$$N_L = b_1 \Sigma x_1 y = 7645225.00$$

$$P_L = b_2 \Sigma x_2 y = 378225.00$$

$$K_L = b_3 \Sigma x_3 y = 32400.00.$$

$\therefore$ Linear effect $= N_L + P_L + K_L = 8055850{\cdot}00$ with 3 $d.f.$

Quadratic effect can be found out as follows :

$$\text{Quadratic effect} = b_0 \Sigma y + b_{11} \Sigma x_1^2 y + b_{22} \Sigma x_2^2 y^*$$

$$+ b_{33} \Sigma x_3^2 y - C.F.$$

$$= 627254{\cdot}84 \text{ with } 3\ d.f.$$

s.s. due to linear interaction effects are got as shown below :

$$b_{12} \Sigma x_1 x_2 y = N_L\ P_L = 31250$$

$$b_{13} \Sigma x_1 x_3 y = N_L\ K_L = 33800$$

$$b_{23} \Sigma x_2 x_3 y = P_L\ K_L = 8450.$$

Sum of squares due to lack of fit in this case is the same as the residual sum of squares, which can be obtained by subtracting the s. s. due to all the effects earlier from the total sum of squares.

Total sum of squares $= 9284573{\cdot}33$ with 14 $d.f.$

$\therefore$ Residual sum of squares $= 527968{\cdot}49$ with 5 $d.f.$

Analysis of Variance Table

Source	*d. f.*	*s. s.*	*M. S. S.*
Linear	3	8055850·00	2685283·33
Quadratic	3	627254·84	209084·94
Interactions	3	73500·00	24500·00
Residual	5	522968·49	105593·70
Total	14	9284573·33	

The equation of the surface fitted through the data is

$$y = 3167{\cdot}89 + 691{\cdot}25\, x_1 + 153{\cdot}75\, x_2 + 45{\cdot}00\, x_3 - 91{\cdot}22 x_1^2 - 202{\cdot}48\, x_2^2 - 37{\cdot}47\, x_3^2 + 62{\cdot}50\, x_1x_2 - 65{\cdot}00\, x_1x_3 - 32{\cdot}50\, x_2x_3.$$

The variances and covariances of the different coefficients come out as below :

$$V(b_o) = \frac{7}{9}\sigma^2, \qquad \text{Cov}\,(b_o, b_{ii}) = -\frac{2}{9}\sigma^2$$

$$V(b_i) = \frac{\sigma^2}{16} \qquad \text{Cov}\,(b_{ii}, b_{jj}) = \frac{17}{288}\sigma^2$$

$$V(b_{ii}) = \frac{13}{144}\sigma^2$$

$$V(b_{ij}) = \frac{\sigma^2}{8}.$$

The response at the central point (0, 0, ... 0) estimated from this design is 3167·89 lbs. The variance of the response is $0{\cdot}7784\sigma^2$. Had the design been rotatable the variance of the response at the central point would have been $0{\cdot}9876\sigma^2$ which is greater than the variance in the case of near rotatable design.

Summary

A series of response surface designs have been obtained along with the derivations of their analysis. These designs can be obtained from the central composite rotatable designs by taking the dose equispaced instead of those required by the rotatable design. It has been shown that these designs are better than the central composite rotatable designs in respect of the precision of estimated response at the central region. The method of analysis has been illustrated through an example.

References

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