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RESEARCH ARTICLE

CONSTRUCTION OF THIRTY-TWO POINTS SPECIFIC OPTIMUM SECOND ORDER ROTATABLE
DESIGNS IN THREE DIMENSIONS WITH A PRACTICAL EXAMPLE

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ABSTRACT

This quadratic response surface methodology focuses on finding the levels of some (coded) predictor variables $\mathbf{x} = (x_{1u}, x_{2u}, x_{3u})'$ that optimize the expected value of a response variable y_u from natural levels. The experiment starts from some best guess or "control" combination of the predictor variables (usually coded to $\mathbf{x} = 0$ for this case $x_{1u}=30$, $x_{2u}=25$ and $x_{3u}=40$) and experiment is performed varying them in a region around this center point. We go further to construct a specific optimum second order rotatable design of three factors in thirty-two points. The achievement of this is done with estimation of the free parameters using calculus in an existing second order rotatable design of thirty-two points. Such a design permits a response surface to be fitted easily and provides spherical information contours besides the realizations of optimum combination of ingredients in Agriculture, horticulture and allied sciences which results in economic use of scarce resources in relevant production processes. The expected second order rotatable design model in three dimensions is available where the responses would then facilitate the estimation of the linear and quadratic coefficients. An example involving Phosphate (x_{1u}), Nitrogen (x_{2u}) and Potassium (x_{3u}) is used to represent the three factors in the coded level and converted into natural levels.

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INTRODUCTION

Response Surface Methodology is a powerful and efficient mathematical approach widely applied in the optimization of cultivation process. The world is facing food shortage and search for alternative or improve measures is inevitable in agricultural fields. Since arable land is a fraction so we need to produce maximally in such areas by utilizing design of experiment like the one design in this study. The main objective of the experimenter is usually to estimate the absolute response or the parameters of a model providing the relationship between the response and the factors. In this context, rotatable designs were introduced by Box and Hunter (1957) in order to explore the response surface. They developed second order rotatable design through geometrical configurations. Draper (1960) says a second order rotatable design aids the fitting of a second order surface and provides spherical information contours. Bose and Draper (1959) point out that the technique of fitting a response surface is one widely used to aid in the statistical analysis of experimental work in which the response of a product depends, in some unknown fashion, on one or more controllable variables. Before the details of such analysis can be carried out, experiments must be performed at predetermined levels of the controllable factors, that is, an experimental design must be selected prior to experimentation.

Draper and Beggs (1971) state that once an experimenter has a polynomial model of suitable order, the problem arises as how best to choose the settings for the independent variables over which he has control. A particular selection of settings or factor levels, at which observations are to be taken is called a design. Designs are usually selected to satisfy some desirable criteria chosen by the experimenter. These criteria include the rotatability criterion and the criterion of minimizing the mean square error of estimation over a given region in the factor space. The present work represents an attempt to meet, in part, this need using the rotatability criterion. Rotatable designs have the nice property that the variance of the estimated response is constant at points equidistant from the centre of the design, conventionally taken to be the origin of the factor space, after transformations if necessary. Rotatable designs generate information about the response surface equally in all directions and are therefore useful when no or little prior knowledge is available about the nature of the response surface. The class of rotatable designs is also very rich in the sense that under many commonly used criteria, such as D-optimality, the optimal designs for polynomial regression models over hyperspherical regions may be found within this class (Kiefer (1960)). Because of the above reasons, a large volume of literature in experimental design is devoted to the investigation of properties and constructional problems of rotatable designs.

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Construction of thirty-two points specific optimum second order rotatable designs in three dimensions

Kosgei *et al.* (2006) gave criteria of selecting the optimality of a design based on known classical optimality criteria. Bose and Draper (1959) define certain transformations applied to points in three dimensions. Let $W(x,y,z)=(y,z,x)$, $W^2=(x,y,z)=(z,x,y)$, $W^3=(x,y,z)=(x,y,z)$, $W^3 = I$ the unit matrix.

Thus I, W, W^2 form a cyclic group of linear transformation in three dimensions.

Further, let $R_1(x,y,z)=(-x,y,z)$, $R_2(x,y,z)=(x,-y,z)$, and $R_3(x,y,z)=(x,y,-z)$, but $R^2_1=R^2_2=R^2_3=I$

The four transformations of coordinates represented by W, R_1, R_2 and R_3 generate a group G of transformations of order 24 with elements

$W^j, W^jR_1, W^jR_2, W^jR_3, W^jR_2R_3, W^jR_3R_1, W^jR_1R_2, W^jR_1R_2R_3, \dots, \dots, (1) (j=1,2,3)$

It is easily seen that all the 24 elements in (1) are distinct. While R_1, R_2 and R_3 commute, W^j and R_j do not ($i, j=1, 2, 3$)

The 24 points of $G(x,y,z)$ will coincide in pairs or in triplets or in quadruplets.

The following is the design of twenty six points that the free parameters f, a, c will be determined

$$D = \left[\frac{1}{2} G(f, f, 0) + \frac{1}{3} G(a, a, a) + \frac{1}{4} G(c, 0, 0) \right] \quad (2.0)$$

We shall consider the above set of thirty-two points from Draper (1960) and Mutiso (1998). The set of thirty-two points in (2.0) form a second order rotatable arrangement in three dimensions if the following moment conditions hold

$$\sum_{u=1}^{32} x_{iu}^2 = 8p^2 + 16q^2 + 8a^2 = 32\lambda_2$$

$$\sum_{u=1}^{32} x_{iu}^4 = 8p^4 + 16q^4 + 8a^4 = 96\lambda_4$$

$$\sum_{u=1}^{32} x_{iu}^2 x_{ju}^2 = 8q^4 + 16p^2 q^2 + 8a^4 = 32\lambda_4$$

(for $i \neq j = 1, 2, 3$) and all other sums of products and powers up to and including order four are zero.

The excess of

$$\sum_{u=1}^{32} x_{iu}^4 = 3 \sum_{u=1}^{32} x_{iu}^2 x_{ju}^2$$

will be denoted by

$$Ex \left\{ G(p, q, q) + \frac{1}{3} G(a, a, a) \right\} = 0$$

therefore

$$\sum_{u=1}^{32} x_{iu}^4 - 3 \sum_{u=1}^{32} x_{iu}^2 x_{ju}^2 = p^4 - q^4 - 48p^2 q^2 - 16a^4 = 0$$

$$8p^4 - 8q^4 - 48p^2 q^2 - 16a^4 = 0$$

$$p^4 - q^4 - 6p^2 q^2 - 2a^4 = 0$$

substituting

$$p^2 = xa^2 \text{ and } q^2 = ya^2$$

$$x^2 - y^2 - 6xy - 2 = 0$$

Implying that $y = \frac{-6x \pm \sqrt{(40x^2 - 8)^2}}{2}$, $\sqrt{2} < x < \infty$

Specifically when $x=15$ then $y=2.413078$ then

$$p^2 = xa^2 = 15a^2 \text{ and } q^2 = ya^2 = 2.413078a^2$$

$$p = 3.872983a \quad q = 1.553409a$$

The points form second order specific rotatable arrangement in three dimensions in the thirty-two points if the non-singularity condition of rotatability

$$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2} \text{ is satisfied}$$

$$\lambda_2 = \frac{1}{32} \sum_{u=1}^{32} x_{iu}^2 = \frac{8(15a^2) + 16(2.413078a^2) + 8a^2}{32}$$

$$\lambda_2 = 5.206539a^2$$

$$\lambda_4 = \frac{1}{32} \sum_{u=1}^{32} x_{iu}^2 x_{ju}^2 =$$

$$\frac{8(2.413078a^2)^2 + 16(2.413078a^2)(15a^2) + 8a^4}{32}$$

$$\lambda_4 = 19.803821a^4$$

$$\frac{\lambda_4}{\lambda_2^2} = \frac{19.803821a^4}{(5.206539a^2)^2} = 0.730551 > \frac{k}{k+2} = 0.6$$

Mutiso(1998) shows that the expansion of $var(y_u)$ is given by

$$var(\hat{y}_u) = \frac{\beta\sigma^2}{N} \left\{ 2(k+2)\beta_2^2 + [(k+2)\beta_2 - (k-1)]3k\beta_2 - 4k\beta_2 - 2(\beta_2 - 1)\beta_2 k(k-1) - \frac{k}{\lambda_2} \frac{\lambda_2 k(k-1)}{\beta_2} \right\}$$

where

$$\beta = [2\beta_2((k+2)\beta_2 - k)]^{-1} \text{ and } \beta_2 = \frac{\lambda_4}{\lambda_2^2} \neq \frac{k}{k+2}$$

$$\beta = 0.953742 \text{ and } \beta_2 = 0.730551$$

$$var(\hat{y}_u) = \frac{0.953742\sigma^2}{32} \{ 9.799387 - 0.576199a^2 - 42.761195a^2 \}$$

$$var(\hat{y}_u) = 0.292065\sigma^2 - 0.017173\sigma^2 a^2 - 1.274473\sigma^2 a^2 = 0$$

$$\frac{\partial(var(\hat{y}_u))}{\partial a} = 0.034346\sigma^2 a^{-3} - 2.548946\sigma^2 a = 0$$

$$\frac{0.034346\sigma^2}{2.548946\sigma^2} = a^4$$

$$a = 0.340705$$

Then $p = 3.872983a = 1.319546$

and $q = 1.553409a = 0.529255$

A Practical Hypothetical Example

A central composite rotatable design was set up to investigate the effects of three fertilizer ingredients on the yield of hybrid maize in Rift Valley to illustrate the use of the specific optimum second order rotatable designs of twenty points under field conditions.

The fertilizer ingredients and actual amount applied were phosphoric acid (P₂O₅) x₁, Ψ₁=30 milligram/hole; Nitrogen (N) x₂ Ψ₂=25 milligram/hole; and potash (K₂O) x₃ Ψ₃=40 milligram/hole. The response of interest is the average yield in mg per hole of hybrid Maize

$$D = \left\{ \begin{aligned} &G(1.319546, 0.529255, 0.529255) + \\ &\frac{1}{3}G(0.340705, 0.340705, 0.340705) \end{aligned} \right\}$$

As a result of soil mapping investigations which indicate deficiencies of these minerals elements in the rift-valley loam soil. The original letters f, a and c represent the variation in quantity application of a factor due to soil fertility gradient culminating in several radii manifestations of rotatability criterion. According to Box(1952) and Box and Wilson (1951) it can be reverted to the natural levels denoted by Ψ_{iu} where Bose and Draper (1959) scaling condition fixes a particular design when λ₂=1 where

$$x_{iu} = \frac{\Psi_{iu} - \Psi_{i\bullet}}{S_i}$$

$$\Psi_{i\bullet} = \frac{\sum_{u=1}^N \Psi_{iu}}{N}$$

$$S_i = \left[\frac{\sum_{u=1}^N (\Psi_{iu} - \Psi_{i\bullet})^2}{N} \right]^{\frac{1}{2}}$$

$$\Psi_{iu} = x_{iu} S_i + \Psi_{i\bullet}$$

For $\sum_{u=1}^N x_{iu}^2 = N$ and $\sum_{u=1}^N x_{iu} = 0$

The value 30mg, 25mg and 40mg/hole represent the centers of the value for Phosphoric acid, Nitrogen and Potash respectively. The design matrix can be constituted but the evaluation of the inverse will be a major computational project to estimate the coefficients of the second order rotatable design model which give the optimum response or yield

Let the scale parameter

S_i, assume s₁=0.5, s₂=0.3 and s₃=1

To estimate the coefficients

β₀, β₁, β₂, β₃, β₁₁, β₂₂, β₃₃, β₁₂, β₁₃ and β₂₃ in the expected second order rotatable design model in three dimensions

$$y_u = \beta_0 x_{0u} + \beta_1 x_{1u} + \beta_2 x_{2u} + \beta_3 x_{3u} + \beta_{11} x_{1u}^2 + \beta_{22} x_{2u}^2 + \beta_{33} x_{3u}^2 + \beta_{12} x_{1u} x_{2u} + \beta_{13} x_{1u} x_{3u} + \beta_{23} x_{2u} x_{3u} + \epsilon_u$$

we require field observation of the yield

$$y_u \quad (u = 1, 2, \dots, 20)$$

The complete second order model to be fitted to yield values is

$$y_u = \beta_0 + \sum_{i=1}^{20} \beta_i x_i + \sum_{i=1}^{20} \beta_{ii} x_i^2 + \sum_{i=1}^{19} \sum_{j=2}^{20} \beta_{ij} x_i x_j + e$$

The following table list the design setting of x₁ x₂ and x₃ and the observed values at 26 design points P₂O₅,N , K₂O and yield are in mg

Coded Values			Natural Values		
(x _{1u}	x _{2u}	x _{3u})	Ψ _{1u}	Ψ _{2u}	Ψ _{3u}
1.319546	0.529255	0.529255	30.659773	25.158777	40.529255
-1.319546	0.529255	0.529255	29.340227	25.158777	40.529255
1.319546	-0.529255	0.529255	30.659773	24.841224	40.529255
1.319546	0.529255	-0.529255	30.659773	25.158777	39.470745
-1.319546	-0.529255	0.529255	29.340227	24.841224	40.529255
-1.319546	0.529255	-0.529255	29.340227	25.158777	39.470745
1.319546	-0.529255	-0.529255	30.659773	24.841224	39.470745
-1.319546	-0.529255	-0.529255	29.340227	24.841224	39.470745
0.529255	0.529255	1.319546	30.264628	25.158777	41.319546
-0.529255	0.529255	1.319546	29.735373	25.158777	41.319546
0.529255	-0.529255	1.319546	30.264628	24.841224	41.319546
0.529255	0.529255	-1.319546	30.264628	25.158777	38.680454
-0.529255	-0.529255	-1.319546	29.735373	24.841224	41.319546
-0.529255	0.529255	-1.319546	29.735373	25.158777	38.680454
0.529255	-0.529255	-1.319546	30.264628	24.841224	38.680454
-0.529255	-0.529255	-1.319546	29.735373	24.841224	38.680454
0.529255	1.319546	0.529255	30.264628	25.395864	40.529255
-0.529255	1.319546	0.529255	29.735373	25.395864	40.529255
0.529255	-1.319546	0.529255	30.264628	24.604136	40.529255
0.529255	1.319546	-0.529255	30.264628	25.395864	39.470745
-0.529255	-1.319546	0.529255	29.735373	24.604136	40.529255
-0.529255	1.319546	-0.529255	29.735373	25.395864	39.470745
0.529255	-1.319546	-0.529255	30.264628	24.604136	39.470745
-0.529255	-1.319546	-0.529255	29.735373	24.604136	39.470745
0.340705	0.340705	0.340705	30.170353	25.102212	40.340705
-0.340705	0.340705	0.340705	29.829648	25.102212	40.340705
0.340705	-0.340705	0.340705	30.170353	24.897789	40.340705
0.340705	0.340705	-0.340705	30.170353	25.102212	39.659295
-0.340705	-0.340705	0.340705	29.829648	24.897789	40.340705
-0.340705	0.340705	-0.340705	29.829648	25.102212	39.659295
0.340705	-0.340705	-0.340705	30.170353	24.897789	39.659295
-0.340705	-0.340705	-0.340705	29.829648	24.897789	39.659295

Applications

Practical application of these methods is not automatic, that judgment is required. It is always possible, especially in a new field of experiment, to make an unfortunate selection of units and again it is solely a question of judgment. This design permits a response surface to be fitted easily and provides spherical information contours besides the realizations of optimum combination of ingredients in Agriculture, horticulture and allied sciences which results in economic use of scarce resources in relevant production processes. The design enable us to see that the specific optimum second order design of three dimensions in twenty six points are met and the expected second order rotatable design model in three dimensions will be available when an experimenter would carry out an experiment where the responses would then facilitate the estimation of the linear and quadratic coefficients.

Conclusion

This study presented a brief overview by utilizing response surface methodology to obtain mathematical parameters of coded values and its corresponding natural levels that can approximate the functional relationship between performance characteristics and design variables. After an experimenter has done the experiment the resulting response is used to construct response surface approximation model using least squares regression analysis. However, in physical experiments there is usually some variability in the output response with the experiment repeated with the same inputs, so it is not automatic, judgment must be applied to get “good” response. Nowadays, the over use of N (Nitrogen) relative to P₂O₅ (Phosphate) and K₂O (Potassium) concerns both from

agronomic and environmental perspective. Phosphate and Potassium fertilizers have been in short supply and farmers have been more steadily adopting the use of nitrogenous fertilizers because of impressive virtual response. There is evidence that soil P_2O_5 and K_2O level are declining. So determining the optimum balance of N, P_2O_5 and K_2O so as to produce high yield of hybrid maize has been an important issue.

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