



A Sequential Third Order Rotatable Design of Eighty Points in Four Dimensions with an Hypothetical Case Study

Nyakundi Omwando Cornelious^{1*} and Matunde Nambilo Cruyff¹

¹Department of Statistics and Computer Science, Moi University, Eldoret, Kenya.

Authors' contributions

This work was carried out in collaboration between both authors. Author NOC designed the study, performed the statistical analysis, wrote the protocol and wrote the first draft of the manuscript. Author MNC managed the analyses of the study and managed the literature searches. Both authors read and approved the final manuscript.

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Abstract

In research, experiments must be performed at pre determined levels of the controllable factors, meaning that an experimental design must be selected before the experiment takes place. Once an experimenter has chosen a polynomial model of suitable order, the problem arises on 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. A design may become inappropriate under special circumstances requiring an increase in factors or levels to make it more desirable. In agriculture for instance, continuous cultivation of crops may exhaust the previously available mineral elements necessitating a sequential appendage of the mineral elements which become deficient in the soil over time.

In current study, an eighty points four dimensional third order rotatable design is constructed by combining two, four dimensional second order rotatable designs and a practical hypothetical case study is given by converting coded levels to natural levels. We present an illustration on how to obtain the mathematical parameters of the coded values and its corresponding natural levels for a third order

*Corresponding author: E-mail: nyakundicornelious@yahoo.com;

rotatable design in four dimensions by utilizing response surface methodology to approximate the functional relationship between the performance characteristics and the design variables. This design permits a response surface to be fitted easily and provides spherical information contours besides the economic use of scarce resources in relevant production processes.

Keywords: Response surface; rotatable designs; third order.

1 Introduction

Response surface methodology (RSM) is a collection of mathematical and statistical techniques useful for analysing problems where several independent variables influence a dependent variable and its objective is to optimize the dependent variable. In recent years, RSM has been widely recognised as a very important tool for use in various fields such as in Medicine, Agriculture and chemical Industry. The Kenyan economy for instance is mainly dependent on agriculture to produce food for both domestic consumption and export. The Kenyan population is growing at an alarming rate but the natural resources especially land which the population depends on have remained constant and minimal. This has necessitated proper utilization of the scarce commodity of land for maximum returns. In the past, unproductive land could be left fallow to naturally regain the exhausted nutrients, but today, the exhausted nutrients are sequentially appended to the soils through the application of deficient elements (fertilizers) courtesy of design of experiments such as RSM. The fitting of the response surface can be complex and costly if done haphazardly thus the process requires expert knowledge on design and analysis of experiments. To cut on costs, an experimenter has to make a choice of the experimental design prior to experimentation. Rotatability is a natural and desirable property, which requires that the variance of a predicted response at a point remains constant at all such points that are equidistant from the design centre. In this context, rotatable designs were introduced by Box and Hunter [1] in order to explore the response surface. They developed second order rotatable designs through geometrical configurations. Bose and Draper [2] 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. Draper and Beggs [3] 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 moment and non-singularity conditions for third order rotatability were derived and developed by Gardiner et al. [4]. They considered a problem arising in the design of experiments for empirically investigating the relationship between a dependent and several independent variables assuming that the form of the functional relationship is unknown but that within the region of interest, the function may be represented by a Taylor series expansion of moderately low order. Draper [5] constructed third order rotatable designs by combining pairs of second order rotatable designs in three dimensions. Draper [6] constructed a third order rotatable design in four dimensions. Mutiso [7] constructed specific and sequential second and third order rotatable designs in three dimensions but did not give the optimality criteria for the designs. Kosgei [8] gave the alphabetic optimality criteria for the designs constructed by Mutiso [7]. Kosgei et al. [9] gave criteria of selecting the optimality of a design based known as classical optimality criteria. Koske et al. [10,11] and Keny et al. [12] constructed optimal second order rotatable designs and gave practical hypothetical examples. Koske and Mutai et al. [13,14,15] used the methods laid down by Huda [4] to construct third order rotatable designs of different factors through balanced incomplete block designs. Cheruiyot [16] evaluated the efficiencies of the six specific second order rotatable designs constructed by Mutiso, [7]. Cornelious [17,18,5] constructed sequential third order rotatable designs in four and five dimensions respectively. Cornelious [19] constructed thirty nine points second order rotatable design in three dimensions with a practical hypothetical example. There is a need to give hypothetical examples to all the existing designs to make them ready for the experimenters to apply in the production processes. The current

study solves, in part, this problem. In this study, we construct a third order rotatable design in four dimensions with eighty points and give a practical hypothetical example to this design.

2 Moments and Non-singularity Conditions for Third Order Rotatability

A set of points is said to form a third order rotatable design in k dimensions if it satisfies the following moment conditions according to Draper [6].

$$\sum_{u=1}^N x_{iu}^2 = A \quad (i=1, 2 \dots k), \quad (1)$$

$$\sum_{u=1}^N x_{iu}^4 = 3 \sum_{u=1}^N x_{iu}^2 x_{ju}^2 = 3C, \quad (2)$$

$$\sum_{u=1}^N x_{iu}^6 = 5 \sum_{u=1}^N x_{iu}^2 x_{ju}^4 = 15 \sum_{u=1}^N x_{iu}^2 x_{ju}^2 x_{lu}^2 = 15D, \quad (3)$$

$$\text{For } i \neq j \neq l = 1, 2, \dots, k, \quad u = 0, 1, \dots, N,$$

And all other sums of powers and products up to order six are zero, where

$$A = N\lambda_2, \quad C = N\lambda_4, \quad \text{and } D = N\lambda_6 \quad (4)$$

The arrangement of points is said to form a rotatable design of third order only if it forms a non-singular third order design (if the points give rise to a non-singular matrix). Gardiner et al. [20] derived the non-singularity conditions as;

$$\begin{aligned} \frac{NC}{A^2} &> \frac{K}{K+2} \\ \frac{AD}{C^2} &> \frac{(K+2)}{(K+4)}. \end{aligned} \quad (5)$$

These are the non-singularity conditions required for a third order rotatable arrangement of points to form third order rotatable designs.

3 Construction of Eighty Points Third Order Rotatable Design in Four Dimensions

The four dimensional third order rotatable design in four dimensions is constructed by combining a pair of second order rotatable design s in four dimensions.

The sets s_1 and s_2 are denoted by,

$$s_1 = [s(a, a, a, a) + s(c_1, 0, 0, 0) + s(c_2, 0, 0, 0)] \quad (6)$$

And

$$s_2 = [s(f, f, 0, 0) + s(a, a, a, a) + s(c, 0, 0, 0)] \quad (7)$$

The combination of s_1 and s_2 gives the four dimensional TORD denoted by,

$$D_4 = [s(a, a, a, a) + s(c_1, 0, 0, 0) + s(c_2, 0, 0, 0) + s(f, f, 0, 0) + s(a, a, a, a) + s(c, 0, 0, 0)] \quad (8)$$

The moments given in 1, 2 and 3 are used on the design points given in 8 to confirm rotatability

These conditions gave,

- i. $c_1^4 + c_2^4 - 16a^4 = 0$
- ii. $c^4 - 16a^4 = 0$
- iii. $c_1^6 + c_2^6 + c^6 + 6f^6 - 224a^6 = 0$
- iv. $f^6 - 16a^6 = 0$ (9)

Solving equation (ii) and (iv) of 9 gave,

$$f^2 = 2a^2 \text{ and } c^2 = 4a^2 \quad (10)$$

Substituting 10 to (iii) of 9 gave,

$$c_1^6 + c_2^6 - 64a^6 = 0 \quad (11)$$

$$\text{Let } c_1^2 = xa^2 \text{ and } c_2^2 = ya^2 \quad (12)$$

Substituting 12 to 11 and (i) of 9 gave,

- i. $x^2 + y^2 = 16$
- ii. $x^3 + y^3 = 64$ (13)

MATLAB software was used to solve equations 13 to obtain,

$$x = 4 \text{ And } y = 0 \quad (14)$$

These finally gave,

$$f^2 = 2.5198421a^2, c_1^2 = 4a^2, c_2^2 = 0 \text{ and } c^2 = 4a^2 \quad (15)$$

where a is arbitrary and has a positive value.

The point set D_4 forms a rotatable arrangement of order three for the values of the constants given in 15.

Substituting 15 to 1 and 2 or 3 gives the values of λ_2, λ_4 and λ_6 which finally satisfies the non-singularity conditions given in 5 hence D_4 forms a third order rotatable design in four dimensions.

4 A Practical Hypothetical Case Study

A design was set up to investigate the effects of four fertilizer ingredients on the yield of hybrid maize in Trans-Nzoia to illustrate the use of the sequential third order rotatable design of hundred and thirty four points in five dimensions under field conditions.

The fertilizer ingredients and actual amount applied were phosphoric acid (p_2o_5) $x_1, \psi_1 = 30$ milligram/hole; Nitrogen (N) $x_2\psi_2 = 25$ milligram/hole; potash (k_2o) $x_3\psi_3 = 40$ milligram/hole and sodium (Na) $x_4\psi_4 = 15$ milligram/hole.

The response of interest is the average yield in mg per hole of hybrid maize.

As a result of soil mapping investigations which indicate deficiencies of these mineral elements in the Trans-Nzoia loam soils, the original letter parameters 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 [1] and Box and Wilson [21] it can be reverted that the natural levels of these mineral elements denoted ψ_{iu} where Bose and Draper [2] scaling down condition fixes a particular design when $\lambda_2 = 1$ hence,

$$x_{iu} = \frac{\psi_{iu} - \psi_i}{s_i} \tag{16}$$

$$\psi_i = \frac{\sum_{u=1}^N \psi_{iu}}{N} \tag{17}$$

$$s_i = \left[\frac{\sum_{u=1}^N (\psi_{iu} - \psi_i)^2}{N} \right]^{0.5} \tag{18}$$

$$\psi_{iu} = x_{iu} s_i + \psi_i \tag{19}$$

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

4.1 An example illustrating the conversion of coded levels to natural levels

Let the natural level $x_{1u} = 0.5$

And the amount of potash applied per hole (ψ_3)= 40milligram/hole

Further let $S=0.3$,

Then using, $\psi_{iu} = x_{iu} s_i + \psi_i$.

$$\psi_{iu} = (0.3 \times 0.5) + 40, \quad \text{thus,}$$

$$\psi_{iu} = 40.15 \text{ milligram/hole}$$

The design matrix can be constituted but the evaluation of the inverse will be a major computational project to estimate the coefficients of the third order rotatable design model which give the optimum response yield. This requires a separate discourse but the actual responses or yields can be obtained if a field experiment is conducted as explained.

Table 1. A summary of the excess functions for hundred and thirty four points TORD in five dimensions

Set composition of class	$s(c_1, 0, 0, 0)$	$s(c_2, 0, 0, 0)$	$s(c, 0, 0, 0)$	$2s(a, a, a, a)$	$s(f, f, 0, 0)$
Number of points	8	8	8	32	24
A_x	$2c_1^2$	$2c_2^2$	$2c^2$	$32a^2$	$12f^2$
E_x	$2c_1^2$	$2c_2^2$	$2c^4$	$-64a^4$	0
H_x	$2c_1^2$	$2c_2^2$	$2c^6$	$-448a^6$	$12f^6$
I_x	0	0	0	$-64a^6$	$4f^6$

Let the scale parameters s_i , assume $s_1=0.5, s_2 = 0.3, s_3=1$ and $s_4 = 0.6$ to estimate the coefficients, we require field observations of the yield $y_u(u=1, 2, \dots, 134)$

The complete third order model to be fitted to yield values is,

$$y_u = \beta_0 + \sum_{i=1}^8 \beta_i x_i + \sum_{i=1}^8 \beta_{ii} x_i^2 + \sum_{i=1}^8 \beta_{iii} x_i^3 + \sum_{i=1}^8 \sum_{j=1}^8 \beta_{ij} x_i x_j + \sum_{i=1}^8 \sum_{j=1}^8 \sum_{l=1}^8 \beta_{ijl} x_i x_j x_l + \sum_{i=1}^8 \sum_{j=1}^8 \beta_{iij} x_i^2 x_j + \sum_{i=1}^8 \sum_{j=1}^8 \beta_{ijj} x_i x_j^2 + e$$

For the hundred and thirty four points third order rotatable design in five dimensions, we have the following coded and natural levels respectively as treatments in the Table 2.

Table 2. A summary of the coded levels and their respective natural levels for S₁ of the TORD in four dimensions

$s_1 = [s(a, a, a, a) + s(c_1, 0,0,0) + s(c_2, 0,0,0)]$

Coded levels				Natural levels			
x_{1u}	x_{2u}	x_{3u}	x_{4u}	ψ_{1u}	ψ_{2u}	ψ_{3u}	ψ_{4u}
1.0	1.0	1.0	1.0	30.5	25.3	41.0	15.6
-1.0	1.0	1.0	1.0	29.5	25.3	41.0	15.6
1.0	-1.0	1.0	1.0	30.5	24.7	41.0	15.6
1.0	1.0	-1.0	1.0	30.5	25.3	39.0	15.6
1.0	1.0	1.0	-1.0	30.5	25.3	41.0	14.4
-1.0	-1.0	1.0	1.0	29.5	24.7	41.0	15.6
-1.0	1.0	-1.0	1.0	29.5	25.3	39.0	15.6
-1.0	1.0	1.0	-1.0	29.5	25.3	41.0	14.4
1.0	-1.0	-1.0	1.0	30.5	24.7	39.0	15.6
1.0	-1.0	1.0	-1.0	30.5	24.7	41.0	14.4
1.0	1.0	-1.0	-1.0	30.5	25.3	39.0	14.4
-1.0	-1.0	-1.0	1.0	29.5	24.7	39.0	15.6
-1.0	-1.0	1.0	-1.0	29.5	24.7	41.0	14.4
-1.0	1.0	-1.0	-1.0	29.5	25.3	39.0	14.4
1.0	-1.0	-1.0	-1.0	30.5	24.7	39.0	14.4
-1.0	-1.0	-1.0	-1.0	29.5	24.7	39.0	14.4
2.0	0.0	0.0	0.0	31.0	25.0	40.0	15.0
-2.0	0.0	0.0	0.0	29.0	25.0	40.0	15.0
0.0	2.0	0.0	0.0	30.0	25.6	40.0	15.0
0.0	-2.0	0.0	0.0	30.0	24.4	40.0	15.0
0.0	0.0	2.0	0.0	30.0	25.0	40.2	15.0
0.0	0.0	-2.0	0.0	30.0	25.0	38.8	15.0
0.0	0.0	0.0	2.0	30.0	25.0	40.0	16.2
0.0	0.0	0.0	-2.0	30.0	25.0	40.0	13.8
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0
0.0	0.0	0.0	0.0	30.0	25.0	40.0	15.0

Table 3. A summary of the coded levels and their respective natural levels for S_2 of the TORD in four dimensions

$$s_2 = [s(f, f, 0, 0) + s(a, a, a, a) + s(c, 0, 0, 0)]$$

Coded levels				Natural levels			
x_{1u}	x_{2u}	x_{3u}	x_{4u}	ψ_{1u}	ψ_{2u}	ψ_{3u}	ψ_{4u}
1.59	1.59	0.00	0.00	30.80	25.50	40.00	15.00
-1.59	1.59	0.00	0.00	29.20	25.50	40.00	15.00
1.59	-1.59	0.00	0.00	30.80	24.50	40.00	15.00
-1.59	-1.59	0.00	0.00	29.20	24.50	40.00	15.00
1.59	0.00	1.59	0.00	30.80	25.00	40.60	15.00
-1.59	0.00	1.59	0.00	29.20	25.00	40.60	15.00
1.59	0.00	-1.59	0.00	30.80	25.00	39.40	15.00
-1.59	0.00	-1.59	0.00	29.20	25.00	39.40	15.00
1.59	0.00	0.00	1.59	30.80	25.00	40.00	16.00
-1.59	0.00	0.00	1.59	29.20	25.00	40.00	16.00
1.59	0.00	0.00	-1.59	30.80	25.00	40.00	14.00
-1.59	0.00	0.00	-1.59	29.20	25.00	40.00	14.00
0.00	1.59	1.59	0.00	30.00	25.50	40.60	15.00
0.00	-1.59	1.59	0.00	30.00	24.50	40.60	15.00
0.00	1.59	-1.59	0.00	30.00	25.50	39.40	15.00
0.00	-1.59	-1.59	0.00	30.00	24.50	39.40	15.00
0.00	1.59	0.00	1.59	30.00	25.50	40.00	16.00
0.00	-1.59	0.00	1.59	30.00	24.50	40.00	16.00
0.00	1.59	0.00	-1.59	30.00	25.50	39.40	14.00
0.00	-1.59	0.00	-1.59	30.00	24.50	39.40	14.00
0.00	0.00	1.59	1.59	30.00	25.00	40.60	16.00
0.00	0.00	1.59	1.59	30.00	25.00	40.60	16.00
0.00	0.00	1.59	1.59	30.00	25.00	40.60	16.00
0.00	0.00	1.59	1.59	30.00	25.00	40.60	16.00
1.00	1.00	1.00	1.00	30.50	25.30	41.00	15.60
-1.00	1.00	1.00	1.00	29.50	25.30	41.00	15.60
1.00	-1.00	1.00	1.00	30.50	24.70	41.00	15.60
1.00	1.00	-1.00	1.00	30.50	25.30	39.00	15.60
1.00	1.00	1.00	-1.00	30.50	25.30	41.00	14.40
-1.00	-1.00	1.00	1.00	29.50	24.70	41.00	15.60
-1.00	1.00	-1.00	1.00	29.50	25.30	39.00	15.60
-1.00	1.00	1.00	-1.00	29.50	25.30	41.00	14.40
1.00	-1.00	-1.00	1.00	30.50	24.70	39.00	15.60
1.00	-1.00	1.00	-1.00	30.50	24.70	41.00	14.40
1.00	1.00	-1.00	-1.00	30.50	25.30	39.00	14.40
-1.00	-1.00	-1.00	1.00	29.50	24.70	39.00	15.60
-1.00	-1.00	1.00	-1.00	29.50	24.70	41.00	14.40
-1.00	1.00	-1.00	-1.00	29.50	25.30	39.00	14.40
1.00	-1.00	-1.00	-1.00	30.50	24.70	39.00	14.40
-1.00	-1.00	-1.00	-1.00	29.50	24.70	39.00	14.40
2.00	0.00	0.00	0.00	31.00	25.00	40.00	15.00
-2.00	0.00	0.00	0.00	29.00	25.00	40.00	15.00
0.00	2.00	0.00	0.00	30.00	25.60	40.00	15.00
0.00	-2.00	0.00	0.00	30.00	24.40	40.00	15.00
0.00	0.00	2.00	0.00	30.00	25.00	40.20	15.00
0.00	0.00	-2.00	0.00	30.00	25.00	38.80	15.00
0.00	0.00	0.00	2.00	30.00	25.00	40.00	16.20
0.00	0.00	0.00	-2.00	30.00	25.00	40.00	13.80

5 Applications

Experiments of this kind are widely applied in the field of agriculture, human medicine, veterinary science and chemical industry to provide useful information. The design under consideration permits a response surface to be fitted easily and provides spherical information contours besides optimum combinations of treatments in agriculture, medicine and industry which results in economic use of scarce resources in relevant production processes. However it is noted that; practical applications of this methods is not automatic, judgement is required, if an experimenter applies insufficient intellect to his results, he is likely to suffer as in any other method of experiment and it is always possible especially in the new field of experiment to make an unfortunate selection of units. The expected third order rotatable design model in four dimensions will be available when an experimenter would carry out an experiment where the responses would facilitate the estimation of the linear, quadratic, interactive and cubic coefficients.

6 Conclusions

The study presented an illustration on how to obtain the mathematical parameters of the coded values and its corresponding natural levels of a third order rotatable design in four dimensions by utilizing response surface methodology to approximate the functional relationship between the performance characteristics and design variables. After experimentation, the resulting response is used to construct response surface approximation model using least squares' regression analysis.

Competing Interests

Authors have declared that no competing interests exist.

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