SOME THIRD ORDER ROTATABLE DESIGNS IN SIX DIMENSIONS

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ABSTRACT

In agriculture, science and technology, experiments must be performed at predetermined levels of the controllable factors, meaning that an experimental design must be selected prior to experimentation. A cyclical group of a certain order in a particular degree of a polynomial forms a rotatable design if it satisfies both moment and non-singularity conditions of the rotatability method or criterion. In agriculture and science, we observe what happens and, based on these observations form a theory as to what may be true, test the theory by further observations, and by experiments and watch to see if the predictions based on the theory are fulfilled. Technology is the application of agricultural and scientific knowledge to practical tasks in all of which statistical theory is crucial in the formulation of theories or hypotheses and evolution of predictions. Suppose an experimenter is interested in determining the relationship between a response and several independent variables. The independent variables may be controlled by the experimenter or observed without control. Suppose, further, that these independent variables represent all the factors that contribute to the response, and that the exact relationship between the response and the independent variables is the response function and, geometrically, it defines a surface called the response surface.

In the real world, however, we rarely know the exact relationship or all the variables which affect that relationship. One way of proceeding then is to graduate, or approximate to, the true relationship by a polynomial function, linear in some unknown parameters to be estimated and of some selected order in the independent variables. Under tentative assumption of the validity of this linear model, which we can justify on the basis of Taylor expansion of the response function, we can perform experiments, fit the model using regression techniques, and then apply standard statistical procedures to determine whether this model appears adequate. Since in practice we do not know all of the factors which affect the response, we usually select a subset of the independent variables which we believe might have significant effects. This selection may be made on the basis of prior knowledge, or a preliminary experiment may be performed to screen the important independent variables out of a larger set of possible independent variables.

Polynomial models of order higher than two are rarely fitted in practice. This is partially because of the difficulty of interpreting the form of the fitted surface which, in any case, produces predictions whose standard errors are greater than those from the lower order fit, and partly because the region of interest is usually chosen small

enough for a first or second order model to be a reasonable choice. Exceptions occur in meteorology, where quite high order polynomials have been fitted, but there are only two or three variables commonly used. When a second order polynomial is not adequate, and often even when it is, the possibility of making a simplifying transformation in response or in one or more of the variables would usually be explored before reluctantly proceeding to higher order, because more parsimonious representations involving fewer terms are generally more desirable. This has limited research in second order polynomials whence the gap in the mathematical world in respect of third order polynomials particularly the development of the mathematical formula for sequential construction in the factors leading to the current endeavour.

Once an experimenter has chosen 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 methods or criteria chosen by the experimenter. These methods or criteria include the rotatability method or criterion and the method or criterion of minimising the mean square error of estimation over a given region in the factor space. The present endeavour represents an attempt to meet, in part, this need in third order polynomial models using the rotatability method or criterion along with the cyclical group of order six to generate the point sets. The criterion or method of rotatability says that the variances of estimates of the response made from the least squares estimates of the Taylor series are constant on circles, spheres or hyperspheres about the centre of the design. Thus, a rotatable design, that is, a design which meets this criterion or method, could be rotated through any angle around its center and the variances of responses estimated from it would be unchanged while the cyclical group of order six generating point sets provides the set of points on which the criterion or method of rotatability is applied.

Specifically, the problem considered is that sequential choice of combinations of levels of independent variables will enable the experimenter to approximate a functional relationship by fitting a Taylor series expansion through terms of order three by the method of least squares and will also follow the criterion or method of rotatability in six factors. Such a sequential choice of combinations of levels of the independent variables will be called a third order rotatable design in six dimensions or factors. The objective is to have eventually the mathematical formulation of third order rotatable designs in a finite number of factors, as is the case for second order rotatable designs. Already in the literature, we have third order rotatable designs in five dimensions or factors but there is no mathematical formula of their sequential construction like we have for second order rotatable designs. This is necessary because when such sequential designs are used, the results of the experiments performed according to the five dimensional designs need not be discarded when appending the sixth factor. In soil science for instance, continuous cultivation of crops

may exhaust previously available mineral elements, necessitating sequential appendage of the mineral elements which become deficient in the soil in time among other examples.

In our endeavour, we were able to append the sixth factor. However, the other aspects of the problem for further study would include the practical field application after the estimation of the free or arbitrary parameters employing the general equivalence theorem, which states that the minimisation of the generalised variance of the estimates of the coefficients which are linear in the polynomial models is equivalent to the minimisation of the maximum variance of the estimated response to identify specific optimum designs of order three and the mathematical formulation for third order rotatability. The moment and the non singularity conditions are by-products of the criterion or method of rotatability which the cyclical group of order six generated points satisfy.

Key words: Five dimensions, rotational designs, sequential, six dimensions, third order

1.0 INTRODUCTION

The technique of fitting a response surface is one widely used, especially in the chemical industry to aid in the statistical analysis of experimental work in which the yield of a product depends, in some unknown fashion, on one or more controllable variables. Before the details of such an analysis can be carried out, experiments must be performed at pre-determined levels of the controllable factors, that is, an experimental design must be selected prior to experimentation, (Bose and Draper ,1959).

Box and Hunter (1957) suggested designs of a certain type, which they called rotatable, as being suitable for such experimentation where the variance of the estimated response is constant at points equidistant from the centre of the design. Such designs permit a response surface to be fitted easily and provide spherical information contours. They geometrically chose the N sets of points at which observations are to be made corresponding to the N points in the space of the variables. Box (1952) discussed the problem arising when it is possible to choose in advance the N combinations of levels at which a set of quantitative factors are to be held in a set of N experiments to determine the slopes of a regression surface assumed planar.

Box and Wilson (1951) and Box (1952), as a means of specifying the extent of variation for a given factor, defined the unit for this variable as

$$S_i = \left[\sum_{u=1}^{N} \frac{(\psi_{iu} - \bar{\psi}_i)^2}{\mathrm{N}} \right]^{1/2}$$ and wrote the design in terms of standardised variables

$$x_{iu} = \frac{\psi_{iu} - \bar{\psi}_i}{S_i}.$$

It will be noted, therefore, that for the standardised variables;

$$\begin{aligned}
&\sum_{u=1}^{N} x_{iu} = 0, \\
&\sum_{u=1}^{N} x_{iu}^2 = N\lambda_2, \\
&\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = 3N\lambda_4, \\
&\sum_{u=1}^{N} x_{iu}^6 = 5\sum_{u=1}^{N} x_{iu}^4 x_{ju}^2 = 15\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 x_{ku}^2 = 15N\lambda_6.
\end{aligned} \qquad (1.0)$$

A second order rotatable design aids the fitting of a second order surface and a third order rotatable design aids the fitting of a third order surface, (Draper, 1960). Herzberg (1967b) found that the variance of the difference between the estimated responses at any two points in the factor space is a function of the distances of the two points from the centre of the design and the angle subtending the points at the centre for a rotatable design.

Box and Wilson (1951) described the experimental attainment of optimum conditions mainly in answer to problems of determining optimum conditions in chemical investigations, but believed that the methods would be of value in other fields where experimentation is sequential and the error fairly small. Gardiner *et al.* (1959) considered a problem arising in the design of experiments for empirically investigating the relationship between a dependent and several independent variables, all variables being continuous. They assumed that the form of the functional relationship is unknown, but that within the range of interest, the function may be represented by a Taylor series expansion of moderately low order. Specifically, they considered that choice of combinations of levels of the independent variables which, one, will enable the experimenter to approximate a functional relationship by fitting a Taylor series expansion through terms of order three, by the method of least squares and, two, will have the property of rotatability.

The problem of fitting a curve to the relationship between the concentration of a stimulus and the proportion of individuals responding probably goes back to Gustav Theodore Fechner who, in 1860, transformed proportions to the corresponding normal deviates for data from psychological experiments. Certainly, Box and Wilson's paper (1951) and the large number of papers by Box and his associates, which followed it in the next decade, constitute the single most powerful source of ideas in the investigation of response surfaces, but many of the fundamental ideas had been used and discussed much earlier as the case of Fechner indicates.

Following on the lines of Huda (1982), Patel and Mutiso (1992) and Koske and Mutiso (2005), we consider the problem of constructing third order rotatable designs in six dimensions from those in five dimensions such that the experiments performed according to the five dimensional designs need not be discarded when analysing the six dimensional designs. The designs constructed allow experiments to be performed sequentially in the factors by starting with experiments involving five factors only. After performing a five dimensional design, the experiments may be stopped if it is felt that the sixth factor is not really needed, while if it is felt that another factor should have been included, the experimenter may proceed by the method presented without discarding the original results. The number of additional experiments required to convert the five dimensional designs into six dimensional designs is smaller than the number of experiments required by the designs with the minimum number of experiments among the available six dimensional third order rotatable designs which are all non-sequential in the factors. The designs presented may therefore be more economical.

2.0 THE CONSTRUCTION OF SIX DIMENSIONAL DESIGNS FROM FIVE DIMENSIONAL DESIGNS

It is known from Box and Hunter (1957); Bose and Carter (1959) and Gardiner, Grandage and Hader (1959) that a set of N points ($N \geq 7$) equally spaced on a circle centred at the origin satisfies the moment requirements of a third order rotatable set and hence, two-dimensional third order rotatable designs may be constructed by combining such point sets associated with two or more distinct circles, Huda (1982).

Huda (1982) constructed three-dimensional third order rotatable designs which share some of the features of the designs constructed by Herzberg (1967a). Patel and Mutiso (1992) extended the work to four -dimensional third order rotatable designs. Koske and Mutiso (2005) recently constructed five-dimensional third order rotatable designs. Suppose such a design is given by the points $(x_{1u}^{(i)}, x_{2u}^{(i)}, x_{3u}^{(i)}, x_{4u}^{(i)}, x_{5u}^{(i)})$ (i=1, 2; u=1,2,...,N) where for each i the points are equally spaced on the hypersphere of radius $\rho_i (i = 1,2)$. Further, let A=$\dfrac{N(\rho_1^2+\rho_2^2)}{5}$,

B=$\dfrac{N(\rho_1^4+\rho_2^4)}{35}$ and C=$\dfrac{N(\rho_1^6+\rho_2^6)}{315}$.

Now, consider a six dimensional point set given by the $2N+230$ points:

$$
\begin{aligned}
&(x_{1u}^{(i)}, x_{2u}^{(i)}, x_{3u}^{(i)}, x_{4u}^{(i)}, x_{5u}^{(i)}, 0) \quad (i = 1,2; u = 1,2,....,N),\\
&(\pm d, 0,0,0,0, \pm b_j) \qquad (j = 1,2,3,4,5,6,7,8),\\
&(0, \pm d, 0,0,0, \pm b_j) \qquad (j = 1,2,3,4,5,6,7,8),\\
&(0,0, \pm d, 0,0, \pm b_j) \qquad (j = 1,2,3,4,5,6,7,8),\\
&(0,0,0, \pm d, 0, \pm b_j) \qquad (j = 1,2,3,4,5,6,7,8),\\
&(0,0,0,0, \pm d, \pm b_j) \qquad (j = 1,2,3,4,5,6,7,8),\\
&(\pm v, \pm v, \pm v, \pm v, \pm v, \pm a),
\end{aligned}
\qquad (2.1)
$$

$$(0,0,0,0,0,\pm\alpha),$$

$$(0,0,0,0,0,\pm\beta),$$

$$(0,0,0,0,0,\pm\gamma).$$

For this set of points the following conditions hold:

$$\sum_{u=1}^{N} x_{mu}^2 = A + 32d^2 + 64v^2 \qquad \text{(m= 1,2,3,4,5)},$$

$$\sum_{u=1}^{N} x_{mu}^4 = 3B + 32d^4 + 64v^4 \qquad \text{(m= 1,2,3,4,5)},$$

$$\sum_{u=1}^{N} x_{mu}^2 x_{nu}^2 = B + 64v^4 \qquad \text{(m‘‘‘n= 1,2,3,4,5)},$$

$$\sum_{u=1}^{N} x_{mu}^6 = 15C + 32d^6 + 64v^6 \qquad \text{(m= 1,2,3,4,5)},$$

$$\sum_{u=1}^{N} x_{mu}^4 x_{nu}^2 = 3C + 64v^6 \qquad \text{(m‘‘‘n= 1,2,3,4,5)},$$

$$\sum_{u=1}^{N} x_{6u}^2 = 20\left(\sum_{j=1}^{8} b_j^2\right) + 64a^2 + 2(\alpha^2 + \beta^2 + \gamma^2),$$

$$\sum_{u=1}^{N} x_{6u}^4 = 20\left(\sum_{j=1}^{8} b_j^4\right) + 64a^4 + 2(\alpha^4 + \beta^4 + \gamma^4),$$

$$\sum_{u=1}^{N} x_{mu}^2 x_{6u}^2 = 4d^2\left(\sum_{j=1}^{8} b_j^2\right) + 64a^2v^2 \qquad \text{(m=1,2,3,4,5)}$$

$$\sum_{u=1}^{N} x_{6u}^{6} = 20(\sum_{j=1}^{8} b_j^6) + 64a^6 + 2(\alpha^6 + \beta^6 + \gamma^6),$$

$$\sum_{u=1}^{N} x_{mu}^{4} x_{6u}^{2} = 4d^4(\sum_{j=1}^{8} b_j^2) + 64a^2v^4 \qquad (m=1,2,3,4,5),$$

$$\sum_{u=1}^{N} x_{mu}^{2} x_{6u}^{4} = 4d^2(\sum_{j=1}^{8} b_j^4) + 64a^4v^2 \qquad (m=1,2,3,4,5)$$

$$\sum_{u=1}^{N} x_{mu}^{2} x_{nu}^{2} x_{6u}^{2} = 64a^2v^4 \qquad (m“‘n=1,2,3,4,5),$$

and all other sums of powers and products up to order six are zero. It follows that this set of points forms a third order rotatable design in six dimensions if:

$$d^2 = 2v^2,$$
$$b_1^2 = ... = b_8^2 = a^2 = \frac{3v^2}{2},$$
$$v^4 = \frac{B}{128}, \qquad (2.2)$$
$$v^6 = \frac{3C}{224},$$

with

$$\alpha^2 + \beta^2 + \gamma^2 = \frac{A - 208v^2}{2},$$

$$\alpha^4 + \beta^4 + \gamma^4 = 36v^4, \qquad (2.3)$$

$$\alpha^6 + \beta^6 + \gamma^6 = 342v^6.$$

Let $\rho_2^2 = t\rho_1^2$ $(t \neq 0,1)$. Then the last two equations in (2.2) are simultaneously satisfied if there exists t such that:

$$\frac{(1+t^2)^3}{(1+t^3)^2} = \frac{162.53968}{N}, \qquad (2.4)$$

and then $v^4 = \dfrac{N(1+t^2)\rho_1^4}{4480}$.

3.0 APPLICATIONS

The levels of the factors in each treatment could either be qualitative or quantitative depending on the nature of the experiment. Once the experiment is carried out, the exact response surface could be fitted using the method of least squares, which can then be used to obtain the levels of the factors at which the response is optimum.

Experiments of this kind are widely conducted in the fields of human medicine, veterinary science and agriculture, providing useful information.

In the discussion on Box and Wilson's paper (1951), Box defined experiments which include all combinations of several different treatments or factors as factorial experiments but it was adopted that all experiments with factors are factorial experiments. Wilson emphasised that the practical application of these methods is not automatic, that judgment is required, and that a bad experimenter suffers here as in any other method of experiment - a bad experimenter being one who is not fully aware of what he does and who applies an insufficient intellect to his results.

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The current endeavour is geared to construct in sequence third order rotatable designs in k factors on the lines of those in second order.

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