Algebraic Foundations of Third Order Rotatability in Two Dimensions

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Abstract

The **mechanisms of some scientific phenomena are understood sufficiently well that useful mathematical models that flow directly from the physical mechanisms can be written down. Such models are not considered in this study. Response surface methodology in Schlaflian vectors and matrices representation for rotatability of experimental design points and optimal design theory in Kronecker product representation for measuring rotatability of experimental design points will be appropriate to the study of phenomena that are presently not sufficiently well understood to permit the mechanistic approach. These two techniques have three kinds of applications one approximate mapping of a surface within a limited region two choice of operating conditions to achieve desired specifications and three search for optimal conditions and are a generalization of factorial designs emphasizing the concept of rotatability. The**

problem of fitting a curve to the relationship between the concentration of a stimulus and the proportion of individuals responding transforming proportions to the corresponding normal deviates for data from psychological experiments is the precursor of these techniques. The concept of rotatability produced very strong reactions and the division between theoretical statisticians researching into the theory of optimal design and practical statisticians designing experiments for applied research workers is still very wide because the assumptions in the theory of optimal design have been restrictive with linear models assumed almost exclusively and the optimality criterion based on the generalized variance of the parameter estimates. This restrictiveness undoubtedly explains some of the reluctance of practical statisticians to try to produce "optimal" designs for practical problems. Development has come about mainly in answer to problems of determining optimum conditions in chemical investigations but the methods will be of value in other fields where experimentation is sequential and the error fairly small. The current endeavor is geared to be of use in deriving some new third order rotatable designs in higher dimensions from some of the available third order rotatable designs in lower dimensions. When these designs are used the results of the experiments performed according to the lower dimensional designs need not be discarded. Some of these designs may be performed sequentially in all factors and require a smaller number of points than most of the available third order rotatable designs. Algebra is used in the current effort and the results support existing moment and non-singularity conditions of third order rotatability hence "algebraic foundations" reference. Designs having a spherical variance insure that the estimated response has

a constant variance at all points which are the same distance from the centre of the design. The unknown functional relationship may be represented by a Taylor series expansion of moderately low order within the region of interest. To get usable third order designs, we must combine at least two spherical sets of points with different positive radii as we have shown in these algebraic foundations of third order rotatability. The technique of fitting a response surface is one widely used 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 predetermined levels of the controllable factors, i.e., an experimental design must be selected prior to experimentation. Rotatable designs permit a response surface to be fitted easily and provide spherical information contours where rotatability is coined from rotation in the multiplication of a vector and an orthogonal matrix when the original vector and the resulting vector have the same magnitude but face different directions from a common centre. In the real world 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 the tentative assumption of the validity of this linear model which we can justify on the basis of Taylor expansion, we can perform experiments, fit the model using regression techniques, and then apply standard statistical procedures to determine whether this model appears adequate. A particular selection of settings, or factor

levels, at which observations are to be taken is called a design. Designs are usually selected to satify some desirable criteria chosen by the experimenter and errors can arise in one or more of the following ways one the true response may be observed with error two the functional relationship may not be the correct model three the observations on the independent variables may contain errors.

Introduction

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 Fechner (1860) who transformed proportions to the corresponding normal deviates for data from psychological experiments. Mead and Pike (1975) pointed out that certainly Box and Wilson's paper of 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. Mead and Pike (1975) further stated that the theory of optimal design produced very strong reactions and the division between theoretical statisticians researching into the theory of optimal design and practical statisticians designing experiments for applied research workers is still very wide because he assumptions in the theory of optimal design have been restrictive as linear models are assumed almost exclusively and the optimality criterion is based on the generalized variance of the parameter estimates. This restrictiveness undoubtedly explains some of the reluctance of practical statisticians to try to produce "Optimal" designs for practical problems. Box and Wilson (1951) described the result of their study extending over few years (Wilson a chemist and Box a statistician) where development came about in answer to problems of determining optimum conditions in chemical investigations, but the believed that the methods would be of value in other fields where experimentation is sequential and the error fairly small. Draper and Beggs (1971) said that in the real world, however, we rarely, know the exact relationship, or all the variables which affect that relationship. One way of proceeding Draper and Beggs (1971) thought then is to graduate, or approximate to, the true relationship by a function, linear in some unknown parameters to be estimated and of some selected order in the independent variables. Draper and Beggs (1971) continued reiterating tht under that tentative assumption of the validity this linear model (which can be justified 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. The errors arise in one or more of the following ways one the true response may be observed with error two the true response function may not be the correct model and three the observations on the independent variables may contain errors. 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 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 according to Draper and Beggs (1971). Response surface techniques are a generalization of factorial designs, emphasizing the concept of rotatability in Schlaflian vectors and matrices representation for rotatability of experimental design points and Kronecker product representation for measuring rotatability of experimental design points.

Box and Draper (1987) distinguished that the mechanisms of some scientific phenomena are understood sufficiently well that useful mathematical models that flow directly from the physical mechanisms can be written down unlike in Schlaflian vectors and matrices representation for rotatability of experimental design points and Knonecker product representation for measuring rotatability of experimental design points. In these two techniques commonly called response surface methodology and optimal design theory the methods will be appropriate to the study of phenomena that are presently not sufficiently well understood to permit the mechanistic approach. These two techniques have three kinds of applications one approximate mapping of a surface within a limited region two choice of operating conditions to achieve desired specifications three search for optimal conditions. When a vector and an orthogonal matrix are multiplied the resulting vector has the same magnitude as the original vector with the two vectors facing different directions from a common centre hence producing rotation

from which the word rotatability is coined. The emphasis in developing rotatable designs has been on the estimation of absolute response rather than of differences in response. The total set of the treatments in the conventional factorial is the set of all combinations of the factors taken at fixed levels and this is the principal governing rotatable designs in respons surface methodology and optimal design theory techniques. Box

and hunter (1957) discussed the problem of experimental design to choose N sets of levels at which observations are to be made and developed moment and non-singularity conditions for second order rotatability. 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 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 and gave both moment and non-singularity conditions of third order rotatability. Draper(1960) argued that experiments must be performed at predetermined levels of the controllable factors i.e., an experimental design must be selected prior to experimentation. Box and Hunter (1957) suggested designs of a certain type, which the called rotatable as being suitable for such experimentation as they permit a response surface to be fitted easily and provide spherical information contours so a third order rotatable design aids the fitting of third order surface and that in order to get usable third order designs, we must combine at least two spherical sets of points with different positive radii, Draper (1960).

Huda (1982a) quoted the third order rotatability conditions as follows from Gardiner etal. (1959) moment conditions

N

(i, j, l = I,…K”), where other sums of powers and products upto order six are Zero. A set of points satisfying these conditions is called a rotatable arrangement of order three. The arrangement is a rotatable design only if it forms a non-singular third order design now with non-singularity conditions

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“If and only if the points lie on two or more spheres centered at the origin of the design according to Draper (1960). Huda (1982b) reviewed earlier works and concluded that a set of N (≤ 7) points equally spaced on a circle centered at the origin satisfies the moment require intents 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 (1982b), Mutiso and Koske (2005 - 2007) and Mutiso and Patel (2010) all made contributions in this area. Suppose such a design is given by the points (x (j) (j), (I = 1, 2 u=1, ….,N) where for each i the points are equally spaced on the circle of radius (=1,1). Further, let

(3) $A= N/2+p_2^{2}),(p$ $B=$
$N/8_1^{4}+p_2^{4})(p$ $C=$
$N/48^{2}+p_2^{6}),(pp$

The current endeavour is of geared to develop algebraic foundations to support these claims. These designs can be performed sequentially and have a minimum number of points.

Theorem

A set of points in two dimensions forms a third order rotatable design if the points are equally spaced on two circles of different radii.

Proof

Suppose such a design is given by the points ($x^{(j)}_{1u}, x^{2}_{2u}$) where for each j the points are equally spaced on the circle of radius p;(j=1,2). We shall initially let.

Summing (7) over dimension k+2, we obtain

Combining the results in (6) and (8), we have

Conclusions and Recommendation

To get usable third order designs, we must combine at least two spherical sets of points with different positive radii.

In view of massive research effort in improving the statistical tools for the investigation of response surfaces, it would be hoped that experimenters would be increasingly using these sophisticated tools in their research work. In the biometria field, at least, te evidence does not support this hope according to Mead and Pike (1975).

These designs allow the experiments to be performed ‘sequentially’ in the factors by starting with experiments involving two factors rather than k factors and this can result in saving of resources. The method described may be extended to construct k dimensional designs which are sequential in the factors. When these designs are used the results of the experiments performed according to the two dimensional designs need not be discarded and require a smaller number of points than most of the available third order rotatable designs. A” the order design permits all the coefficients in a polynomial of order ”d” to be estimated. Further effort is required to shed more light on certain aspects.

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