MULTI-FACTOR EXPERIMENTAL DESIGNS FOR EXPLORING RESPONSE SURFACES[1]

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Summary. Suppose that a relationship $\eta = \varphi(\xi_1, \xi_2, \cdots, \xi_k)$ exists between a *response* η and the levels $\xi_1, \xi_2, \cdots, \xi_k$ of k quantitative *variables* or *factors*, and that nothing is assumed about the function φ except that, within a limited region of immediate interest in the space of the variables, it can be adequately represented by a polynomial of degree d.

A k-dimensional experimental design of order d is a set of N points in the k-dimensional space of the variables so chosen that, using the data generated by making one observation at each of the points, all the coefficients in the dth degree polynomial can be estimated.

The problem of selecting practically useful designs is discussed, and in this connection the concept of the *variance function* for an experimental design is introduced. Reasons are advanced for preferring designs having a "spherical" or nearly "spherical" variance function. Such designs insure that the estimated response has a constant variance at all points which are the same distance from the center of the design. Designs having this property are called *rotatable designs*. When such arrangements are submitted to rotation about the fixed center, the variances and covariances of the estimated coefficients in the fitted series remain constant.

Rotatable designs having satisfactory variance functions are given for $d = 1$, 2; and $k = 2, 3, \cdots, \infty$. Blocking arrangements are derived. The simplification in the form of the confidence region for a stationary point resulting from the use of a second order rotatable design is discussed.

1. Introduction. Suppose we have k *variables* or *factors* whose levels are denoted by $\xi_1, \xi_2, \cdots, \xi_k$ on which depend the level of some response η in accordance with an unknown relationship

$$\eta = \varphi(\xi_1, \xi_2, \cdots, \xi_k). \tag{1}$$

Suppose that in order to explore this relationship, N experiments are performed. The uth of these experiments consists in adjusting the factor levels to a certain set of k predecided values, $\xi_{1u}, \xi_{2u}, \cdots, \xi_{ku}$ and of observing a response y_u. The problem of experimental design discussed is that of choosing the N sets of levels at which observations are to be made. It is often convenient to view the problem geometrically and to regard Eq. (1) as defining a surface referred to as the *response surface*. The N sets of conditions at which the response is observed

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will then correspond to N points in the space of the variables called *experimental points*.

1.1 *Notation.* Following the convention adopted in previous papers [1], [2] we shall define a set of standardized levels

$$x_{iu} = \frac{(\xi_{iu} - \bar{\xi}_i)}{S_i}, \quad \text{where} \quad S_i = \left\{ \sum_{u=1}^{N} \frac{(\xi_{iu} - \bar{\xi}_i)^2}{N/c} \right\}^{1/2} \tag{2}$$

For these standardized levels therefore

$$\sum_{u=1}^{N} x_{iu} = 0 \quad \text{and} \quad \sum_{u=1}^{N} x_{iu}^2 = \frac{N}{c} \tag{3}$$

and for the time being the convention is adopted that $c = 1$.

We shall denote by $\mathbf{D}$ the $N \times k$ *design matrix* which provides a program of the N experiments to be performed. The elements of the uth row of this matrix are the values of the standardized levels $x_{1u}, x_{2u}, \cdots, x_{ku}$ to be used in the uth experiment. These elements also define the uth experimental point in the k-dimensional space of the variables. Since the designs we consider may include many factors, they will be called *multi-factor* designs.

Using standardized factor levels in accordance with Eq. (3) we can prepare standard design matrices appropriate for various values of k, and for various types of assumptions concerning the function φ. In given circumstances the experimenter can select the appropriate design matrix and choose suitable average values $\bar{\xi}_1, \bar{\xi}_2, \cdots, \bar{\xi}_k$ and units $S_1, S_2, \cdots, S_k$ so that the design covers the region of immediate interest in the space of the variables. The level of the ith factor to be used in the uth trial is then $\xi_{iu} = \bar{\xi}_i + S_i x_{iu}$.

We shall assume in what follows that in the limited region of immediate interest φ can be represented by a polynomial of degree d so that the response at the uth point is assumed to be

$$\begin{aligned} \eta_u = {} & \beta_0 x_{0u} + \beta_1 x_{1u} + \cdots + \beta_k x_{ku} + \beta_{11} x_{1u}^2 + \cdots + \beta_{kk} x_{ku}^2 + \cdots \\ & + \beta_{12} x_{1u} x_{2u} + \cdots + \beta_{k-1,k} x_{k-1,u} x_{ku} + \beta_{111} x_{1u}^3 + \text{etc.} \end{aligned} \tag{4}$$

Following convention, we call x_0 ; $x_1, \cdots, x_k$; $x_1^2, \cdots, x_k^2$; $x_1 x_2, \cdots$ etc., the "independent" variables. When the polynomial is of degree higher than the first, the "independent" variables are not, of course, *functionally* independent.

We shall obtain least squares estimates b_0, b_1, etc., of the coefficients β_0, β_1, etc, by fitting Eq. (4) to the N observed values $y_1, y_2, \cdots, y_u, \cdots, y_N$. It is convenient to write down the constant term as $\beta_0 x_{0u}$ rather than as β_0 defining x_{0u} as unity for all values of u. We call β_i the ith *linear* coefficient, β_{ii} the ith *quadratic* coefficient, β_{ij} the ijth *linear* $\times$ *linear crossproduct* coefficient (or simply the ijth interaction coefficient where no ambiguity will arise) and so on. The independent variables $x_i, x_i^2, x_i x_j$ are similarly named.

A design which includes k variables and allows all constants up to order d to be determined will be called a k-dimensional design of order d. In a polynomial equation of degree d there are $\binom{k+d}{d}$ terms, so that for a k-dimensional design of order d, the number of experimental points must be at least $\binom{k+d}{d}$.

1.2 *Factorial designs.* A factorial design from which are to be determined all the polynomial coefficients of order d or less includes all combinations of $d + 1$ levels of each of the factors. The number $(d + 1)^k$ of experimental points so generated is often excessively large compared with the number $\binom{k+d}{d}$ of constants to be determined. In five variables for instance, the factorial design would require $3^5 = 243$ points to determine the 21 constants in the second order polynomial. The number of experimental points may sometimes be considerably reduced by fractional replication [3]. Unfortunately the device of fractional replication is not very effective in generating from the higher level factorials satisfactory designs of order greater than one. For the particular problem here considered of fitting multivariate polynomials to data there seems to be no reason for basing experimental arrangements on the factorials and a more fundamental approach will be attempted.

1.3 *Requirements.* The following are properties of an experimental design of order d which are desirable in the present context. The relative importance of these properties depends on the particular experimental situation. To be of value for specific purposes a design will not need to possess them all.

(a) The design should allow the approximating polynomial of degree d (tentatively assumed to be representationally adequate) to be estimated with satisfactory accuracy within the region of interest.

(b) It should allow a check to be made on the representational accuracy of the assumed polynomial.

(c) It should not contain an excessively large number of experimental points.

(d) It should lend itself to 'blocking'.

(e) It should form a nucleus from which a satisfactory design of order $d + 1$ can be built in case the assumed degree of polynomial proves inadequate.

In this paper we are concerned with interpreting (a) in such a way as, where possible, to satisfy the other properties also. In Section 2 some general results in Least Squares are stated. In Section 3 the criterion of orthogonality is discussed. In Section 4 the concept of the *variance function* for the designs is introduced. This indicates the desirability of designs for which the variance is constant at a constant distance from the origin of the design. Such designs are called *rotatable* designs and the conditions that such designs must satisfy are derived in Sections 5 and 6. In Section 7 second order rotatable designs are obtained. The arrangement into blocks of second order rotatable designs is discussed in Section 8. The details of the calculations required when using the designs is given in Section 9. Completely worked numerical examples will appear in [14]. Section 10 discusses the construction of a confidence region for a stationary point.

2. Least squares results. For any linear model, such as (4), in which there are L unknown coefficients, the N equations at the N experimental points may be written in an obvious matrix notation as

$$\boldsymbol{\eta} = \mathbf{X}\boldsymbol{\beta}, \tag{4a}$$

where the $N \times L$ matrix $\mathbf{X}$ is called the matrix of independent variables.

If the observed values found at the N experimental points are represented by a vector $\mathbf{Y}$ and

$$\mathcal{E}(\mathbf{Y}) = \boldsymbol{\eta}; \qquad \mathcal{E}(\mathbf{Y} - \boldsymbol{\eta})(\mathbf{Y} - \boldsymbol{\eta})' = \mathbf{I}_N\sigma^2 \tag{5}$$

then, on the supposition that the mathematical model (4a) exactly represents the true situation, the estimates $\mathbf{B}$ of $\boldsymbol{\beta}$ linear in the observations which are unbiased (i.e., $\mathcal{E}(\mathbf{B}) = \boldsymbol{\beta}$) and have severally the smallest possible variances, are those which reduce to a minimum the sums of squares of discrepancies $(\hat{\mathbf{Y}} - \mathbf{Y})'(\hat{\mathbf{Y}} - \mathbf{Y})$ between the observed values $\mathbf{Y}$ and the values $\hat{\mathbf{Y}} = \mathbf{XB}$ given by the fitted function. These are the "least squares" estimates

$$\mathbf{B} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}. \tag{6}$$

Their variances and co-variances are the elements of the matrix

$$\mathcal{E}(\mathbf{B} - \boldsymbol{\beta})(\mathbf{B} - \boldsymbol{\beta})' = (\mathbf{X}'\mathbf{X})^{-1}\sigma^2 \tag{7}$$

and an unbiased estimate of $(N - L)\sigma^2$ is provided by the quantity

$$(\hat{\mathbf{Y}} - \mathbf{Y})'(\hat{\mathbf{Y}} - \mathbf{Y}) = \mathbf{Y}'\mathbf{Y} - \mathbf{B}'\mathbf{X}'\mathbf{X}\mathbf{B}. \tag{8}$$

If, contrary to supposition, the mathematical model $\boldsymbol{\eta} = \mathbf{X}\boldsymbol{\beta}$ is inadequate and in fact L_1 further terms $\mathbf{X}_1\boldsymbol{\beta}_1$ are needed to ensure an adequate representation of the response so that

$$\boldsymbol{\eta} = \mathbf{X}\boldsymbol{\beta} + \mathbf{X}_1\boldsymbol{\beta}_1,$$

then the estimates given by (6) are biased for

$$\mathcal{E}(\mathbf{B}) = \boldsymbol{\beta} + \mathbf{A}\boldsymbol{\beta}_1, \tag{8a}$$

where $\mathbf{A} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}_1$ is an $L \times L_1$ matrix of bias coefficients which has been called, [1], the "alias" matrix. In this situation the residual sum of squares is also biased and we find

$$\begin{aligned} \mathcal{E}(\mathbf{Y}'\mathbf{Y} - \mathbf{B}'\mathbf{X}'\mathbf{X}\mathbf{B}) &= (N - L)\sigma^2 + \boldsymbol{\beta}_1'(\mathbf{X}_1 - \mathbf{X}\mathbf{A})'(\mathbf{X}_1 - \mathbf{X}\mathbf{A})\boldsymbol{\beta}_1 \\ &= (N - L)\sigma^2 + \boldsymbol{\beta}_1'\mathbf{X}_1'(\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}')\mathbf{X}_1\boldsymbol{\beta}_1. \end{aligned} \tag{8b}$$

2.1 *The moment matrix.* Equations (6), (7), (8), (8a), and (8b) contain the matrix $\mathbf{X}'\mathbf{X}$ of sums of squares and products of the independent variables. We notice that $N^{-1}\mathbf{X}'\mathbf{X}$ may be viewed as a matrix of *moments* of the design. For example, if there are $k = 2$ variables, and we are considering a design of order two, the equation to be fitted is

(9) $$\eta = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2$$

and the matrix $N^{-1}\mathbf{X}'\mathbf{X}$ is

(10) $$\begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 11 \\ 22 \\ 12 \end{array} \begin{array}{c} \begin{array}{cccccc} 0 & 1 & 2 & 11 & 22 & 12 \end{array} \\ \left[\begin{array}{cccccc} 1 & [1] & [2] & [11] & [22] & [12] \\ [1] & [11] & [12] & [111] & [122] & [112] \\ [2] & [12] & [22] & [112] & [222] & [122] \\ [11] & [111] & [112] & [1111] & [1122] & [1112] \\ [22] & [122] & [222] & [1122] & [2222] & [1222] \\ [12] & [112] & [122] & [1112] & [1222] & [1122] \end{array} \right] \end{array}.$$

The quantities in square brackets denote the moments of the design. For example, $N^{-1}\sum_{u=1}^{N} x_{1u} = [1]$, $N^{-1} \sum_{u=1}^{N} x_{1u}^2 x_{2u} = [112]$ and so on. We shall call $N^{-1}\mathbf{X}'\mathbf{X}$ the moment matrix and its inverse $N(\mathbf{X}'\mathbf{X})^{-1}$ the *precision* matrix. When $\sigma^2 = 1$ the elements of this latter matrix are the variances and covariances of the effects measured on a "per-observation" basis.

3. Orthogonal designs. The problem of choosing a "best" design for the fitting of a model $\boldsymbol{\eta} = \mathbf{X}\boldsymbol{\beta}$ has usually been interpreted as that of satisfying the requirement that $\mathbf{D}$ should be so chosen that the coefficients $\boldsymbol{\beta}$ are separately estimated with smallest variance. In references [4], [5], [2], and [6] a theorem is proved (for the case where the variables in the matrix $\mathbf{X}$ are functionally independent and the diagonal elements of $\mathbf{X}'\mathbf{X}$ are fixed by the definition of the problem) that the requirement of smallest variance is satisfied by so choosing $\mathbf{D}$ that the matrix $\mathbf{X}'\mathbf{X}$ is diagonal. Such an arrangement may be called an orthogonal design.

In the present context it is only in the case of designs of first order that the variables are functionally independent and that all the diagonal elements of $\mathbf{X}'\mathbf{X}$ are fixed by the definition of the problem. For this reason, as we see in more detail below, the above theorem is directly helpful only in the derivation of first order designs. For higher order designs an alternative approach is necessary.

3.1 *First order designs.* In this case the independent variables are $x_0, x_1, \cdots, x_k$. Since these variables are also functionally independent, and since $\sum x_{iu}^2 = N$ $(i = 0, 1, 2, \cdots, k)$ so that the diagonal elements of $\mathbf{X}'\mathbf{X}$ are fixed by definition of the problem, the smallest variance theorem referred to above leads at once to the conclusion that a best design matrix $\mathbf{D}$ is one for which $N^{-1}\mathbf{X}'\mathbf{X} = \mathbf{I}$. It will be noted that for this case we are led to a unique form of moment matrix. Such a moment matrix is realized in practice simply by choosing $\mathbf{D}$ to have orthogonal columns subject to Eqs. (3).

The construction and properties of such designs are discussed in [2]. Geometrically the designs consist of N points, at the vertices of an $N - 1$ dimensional regular simplex if $k = N - 1$, or the projections onto a space of k dimensions of the vertices of the $N - 1$ dimensional regular simplex if $k < (N - 1)$. The arbitrariness in the choice of $\mathbf{D}$ corresponds to the fact that the simplex may be taken in any orientation. This class of designs includes the factorials and fractional factorials. These latter designs are of special value because they are easy to carry out, they allow the adequacy of the first degree representation to be checked and the nature of departures from it to be readily identified, they form natural nuclei which can be augmented to form designs of higher order, and they are readily arranged in blocks.

3.2 *Second order "orthogonal" designs.* For designs of order higher than the first the quantities x_0 ; $x_1, \cdots, x_k$; $x_1^2, \cdots, x_k^2$; $x_1x_2, x_1x_3, \cdots, x_{k-1}x_k$; x_1^3, etc., are not all functionally independent and a diagonal moment matrix is impossible of attainment since, unless the x_{iu} are all zero, certain sums of products such as those between x_i^2 and x_0 and between x_i^2 and x_j^2 are necessarily positive.

Orthogonal second order designs of a sort can be obtained if we redefine the independent variables in terms of the orthogonal polynomials. We show below however that there is an infinite variety of such designs with widely different properties and that these designs do not provide a wholly satisfactory solution to our problem.

Let $x_i^{(m)}$ be the orthogonal polynomial of mth degree for the ith variable x_i. Thus

$$x_i^{(m)} = x_i^m + \alpha_{m-1,m}x_i^{m-1} + \cdots + \alpha_{1m}x_i + \alpha_{0m}, \tag{11}$$

where the α's are chosen so that

$$\sum_{u=1}^{N} x_{iu}^{(m)}x_{iu}^{(m-p)} = 0, \qquad p = 1, 2, \cdots, m. \tag{12}$$

Then we can express the original polynomial equations in terms of these orthogonal polynomials and their products in the form

$$\mathfrak{n} = (\mathbf{XP})(\mathbf{P}^{-1}\boldsymbol{\beta}) = \dot{\mathbf{X}}\dot{\boldsymbol{\beta}},$$

where $\mathbf{P}$ is the matrix transforming the old independent variables to the new. For clarity we will discuss the particular case of a two dimensional design of order 2 but, as will be readily appreciated, the conclusions drawn will be quite general.

Using (3) with (11) and (12) we have

$$x_i^{(1)} = x_i, \; x_i^{(2)} = x_i^2 - [iii]x_i - 1 \tag{13}$$

and the second degree equation (9) for $k = 2$ could be written as

$$\begin{aligned}\eta = {} & (\beta_0 + \beta_{11} + \beta_{22})\, x_0 + (\beta_1 + [111]\,\beta_{11})x_1 + (\beta_2 + [222]\beta_{22})x_2 \\ & + \beta_{11}(x_1^2 - [111]x_1 - 1) + \beta_{22}(x_2^2 - [222]x_2 - 1) + \beta_{12}x_1x_2 .\end{aligned} \tag{14}$$

The symmetric moment matrix $N^{-1}\,\dot{\mathbf{X}}'\dot{\mathbf{X}}$ is then that given below.

$$
(15) \qquad
\begin{array}{c|cccccc|}
 & 0 & 1 & 2 & 11 & 22 & 12 \\
0 & 1 & \cdot & \cdot & \cdot & \cdot & a \\
1 & \cdot & 1 & a & \cdot & b & c \\
2 & \cdot & a & 1 & d & \cdot & e \\
11 & \cdot & \cdot & d & f & g & h \\
22 & \cdot & b & \cdot & g & i & j \\
12 & a & c & e & h & j & k
\end{array}
$$

Here $a = [12]$, $b = [122] - [222][12]$, $c = [112]$, $d = [112] - [111][12]$,

$e = [122], f = [1111] - [111]^2 - 1,$

$g = [1122] + [111][222][12] - [111][122] - [222][112] - 1,$

$h = [1112] - [111][112] - [12], i = [2222] - [222]^2 - 1,$

$j = [1222] - [222][122] - [12], k = [1122].$

To obtain a diagonal matrix we must evidently choose the design so that

$$[12] = [112] = [122] = [1112] = [1222] = 0 \quad \text{and} \quad [1122] = 1,$$

which insures that all the elements of the matrix (15) vanish except those on the diagonal. Examples of such designs are the factorials with more than two levels and the orthogonal composite designs given by Box and Wilson [1].

There seems little justification for limiting consideration to only these arrangements. In particular nothing in our discussion has indicated that the choice $[1122] = 1$ is necessarily a good one, or that it would not be better to choose some other value and let the quadratic effects be correlated. Again, it is far from clear what constitutes a "good" choice of the diagonal elements $[iiii] - [iii]^2 - 1$ corresponding to the quadratic constants in the moment matrix.

Since the scaling of the design has been *standardized*, $[iii]^2$ and $[iiii]$ are measures of "skewness" and "kurtosis" for the ith variable. The choice of the moments $[iii]$ decides the question of whether the marginal distribution of the pattern of design points for ith variable is to be symmetric or skew. The choice of the moments $[iiii]$ decides whether there is to be a tendency to a uniform distribution of points or to a concentration of points at the center and at the extremes of the range. Since for all such designs in our conventional scaling the variances of linear, quadratic and interaction estimates corresponding to the ith variable are σ^2N^{-1}, $\sigma^2N^{-1}([iiii] - [iii]^2 - 1)^{-1}$ and σ^2N^{-1} respectively this choice also decides the relative precision with which linear quadratic and interaction coefficients are estimated.

It may be noted for example that, for the 3^k factorial design in conventional scaling, $[iii] = 0$ and $[iiii] = \frac{3}{2}$ $(i = 1, 2, \cdots, k)$. The variances of the estimates for the quadratic coefficients are thus twice as large as those for the interaction coefficients. In terms of estimated derivatives at the center of the design therefore, the estimated "quadratic" derivative $\partial^2\eta/(\partial x_i)^2$ has *eight times* the variance of the estimated "interaction" derivative $\partial^2\eta/\partial x_i\partial x_j$. This was pointed out in [1], where an intuitive attempt to reduce this apparent unbalance was made by introducing designs in which quadratic and interaction derivatives were determined with equal precision. In fact designs both orothogonal and non-orthogonal can be found for which the relative variances of estimated coefficients of different kinds can differ over a wide range. Up to this point the present discussion has provided no satisfactory basis on which a rational choice can be made.

In selecting from possible orthogonal designs it seems at first sight that the quantities $[iiii] - [ii]^2 - 1$ should be made as large as possible. This would seem to give the smallest possible variances for the quadratic effects without affecting the precision of the remaining constants. On closer inspection however the apparent advantage of such a choice turns out to be somewhat illusory because

(a) The apparent advantage of making the quantity $[iiii] - [ii]^2 - 1$ large arises only because of the particular scale convention adopted. If for example we scaled our designs on the basis of the size of the fourth moment instead of on the size of the second moment a contrary conclusion would be reached.

(b) The quantity $[iiii]$ enters not only into the precision matrix but also into the alias matrix. In fact for any orthogonal design of this type the expected value of the ith linear effect is

$$\mathcal{E}(b_i) = \beta_i + [iiii]\,\beta_{iii} + \sum_{j \neq i}^{k} \beta_{ijj}.$$

Thus the apparent reduction in the variance of the quadratic effects is gained only at the expense of an increase in possible bias in the linear effects.

(c) The quadratic effect β_{ii} measures curvature of the surface in the direction of the ith coordinate axis. It is shown in the next section that by attempting to measure the precision with which curvature is determined in the directions of the coordinate axes we may decrease the precision with which it is determined in some other direction which might be of equal importance to the experimenter.

3.3 *Effect of rotation on precision of the estimates.* If, as we shall assume, we wish to use the design to explore a surface about which little is known, we shall in particular not know how the design is oriented relative to the response surface. For example suppose the surface could be represented locally by an equation of second degree, then the response contours would be a set of conics which could be referred to their principal axes. The orientation of these axes relative to the axes of the variables would differ from one problem to another. It is of some interest therefore to consider how the variances and co-variances of the estimated coefficients are changed when the design is rotated.

As an example suppose that we were to use the symmetrical 3^2 factorial design to estimate the coefficients in the second degree Eq. (9). Then bearing in mind the conventions expressed by Eqs. (3) concerning the origin of the design and the size of the scale factor, we should use the nine combinations of the levels

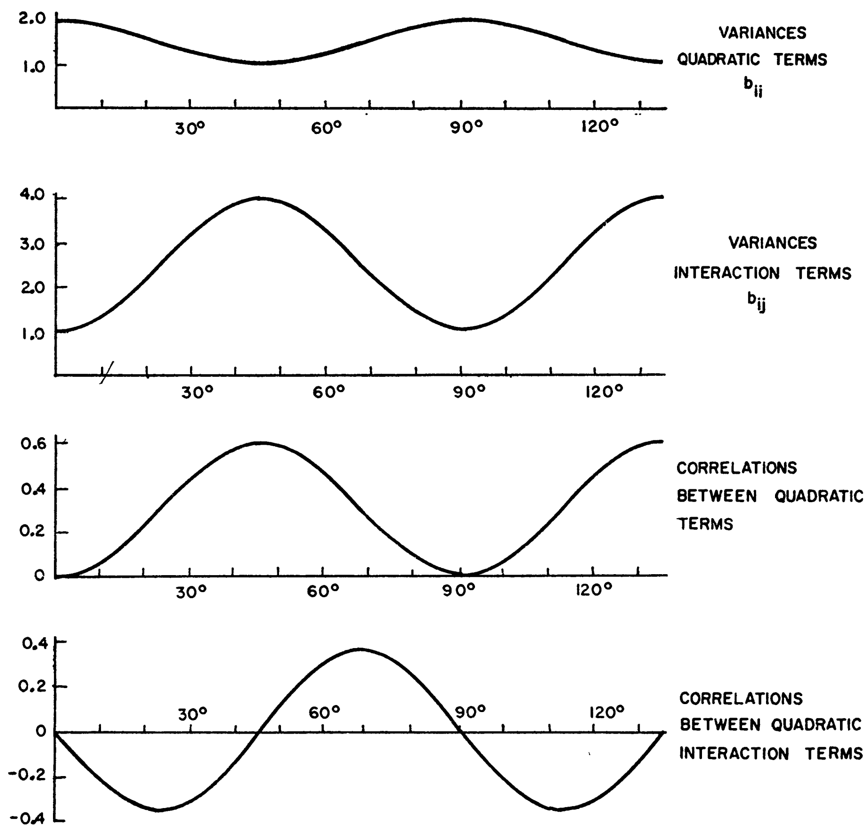

FIG. 1. Variances of, and correlations between, second order coefficients estimated from a 3^2 factorial design rotated through an angle θ

$x_1 = (-\alpha, 0, \alpha)$ and $x_2 = (-\alpha, 0, \alpha)$, where $\alpha = (\frac{3}{2})^{\frac{1}{2}}$. In the normal orientation of the design the variances of the linear effects, quadratic effects and interaction effects would be $\sigma^2/9$, $2\sigma^2/9$ and $\sigma^2/9$ respectively, and consequently the corresponding entries in the precision matrix (which measure the variance on a "per observation" basis for unit experimental error variance) would be 1, 2, and 1, respectively. All the covariances between these effects would be zero. If the design were rotated through some angle θ however then, as is illustrated in Fig. 1 the variances of the quadratic and interaction effects would undergo marked changes and the quadratic effects would become correlated with each other and with the interaction effect. Only the linear effects would have constant variance and would remain unchanged in all orientations.

We see that the variances of individual coefficients estimated using a design in a particular orientation may give a somewhat misleading impression of its efficiency. The condition of orthogonality refers to orthogonality in a particular orientation, and this property is in general lost on rotation of the design.

4. The variance function for the design. We have proceeded so far by considering the accuracy with which *individual* coefficients are estimated. This approach does not, for the case of designs of order higher than the first, seem to lead to any unique class of solutions, but points to the conclusion that we should in some way consider the joint accuracy of the coefficients. We are really interested in the individual coefficients only in so far as they supply information about the surface. To make further progress therefore we consider what we call the design "variance function".

We shall denote the k coordinates $x_1, \cdots, x_i, \cdots, x_k$ of a point in the space of the variables by the $k \times 1$ vector $\mathbf{x} = \{x_i\}$. Suppose that $\hat{y}_x$ is the response estimated at the point $\mathbf{x}$ using a polynomial fitted by least squares to N observations made in accordance with some experimental design $\mathbf{D}$. The variance $V(\hat{y}_x)$ of this estimated value is a function of $\mathbf{x}$ and σ^2 and we can reduce $V(\hat{y}_x)$ by increasing N (for example by replicating the points). The quantity $V(\mathbf{x}) = NV(\hat{y}_x)/\sigma^2$, or alternatively its reciprocal $W(\mathbf{x}) = \sigma^2/NV(\hat{y}_x)$, is thus a standardized measure of the accuracy with which the design $\mathbf{D}$ allows the response at the point $\mathbf{x}$ to be estimated. $NV(\hat{y}_x)/\sigma^2$ will be called the *variance function* of the design and $W(\mathbf{x}) = \{V(\mathbf{x})\}^{-1}$ the *weight function*. For any experimental design $V(\mathbf{x})$ provides a standardized measure of the precision of the estimated response at any point in the space of the variables. It is a function of $x_1, x_2, \cdots, x_k$ and the elements of the precision matrix alone and is uniquely defined for every k dimensional experimental design of order d.

For example suppose we used the nine points of the 3^2 symmetrical factorial as a second order two dimensional design. On the convention that the origin and scale are chosen so that $[1] = [2] = 0$ and $[11] = [22] = 1$, we have for the variances and covariances of the effects $V(b_0) = (\frac{5}{9})\sigma^2$, $V(b_1) = V(b_2) = (\frac{1}{9})\sigma^2$, $V(b_{11}) = V(b_{22}) = (\frac{2}{9})\sigma^2$, $V(b_{12}) = (\frac{1}{9})\sigma^2$ and Cov (b_0b_{11}) = Cov (b_0b_{22}) = $(-\frac{2}{9})\sigma^2$. The variance function for this design is therefore

$$V(\mathbf{x}) = \frac{N}{\sigma^2} V(\hat{y}_x) = 5 - 3x_1^2 - 3x_2^2 + 2x_1^4 + 2x_2^4 + x_1^2x_2^2 .$$

The variance contours for which are shown in Fig. 2(i).

In Figs. 2(ii) and 2(iii) are shown variance functions for other two-dimensional second order designs mentioned in [1]. The arrangement in figure 2(ii) is the "pentagonal design" and that in figure 2(iii) is an example of a class of designs, already referred to in Section 3.2, in which quadratic and interaction *derivatives* are determined with equal precision. It will be seen that the arrangement of points in the latter design is in fact almost the same as would be obtained by rotating the factorial through 45°.

If, as we shall suppose, nothing is known in advance about the orientation of the surface, it seems most appropriate to adopt designs which have variance functions like that of the pentagonal design. That is to say designs which generate information such that the response is estimated with constant variance at all points equidistant from the origin of the design. When we have no knowledge in

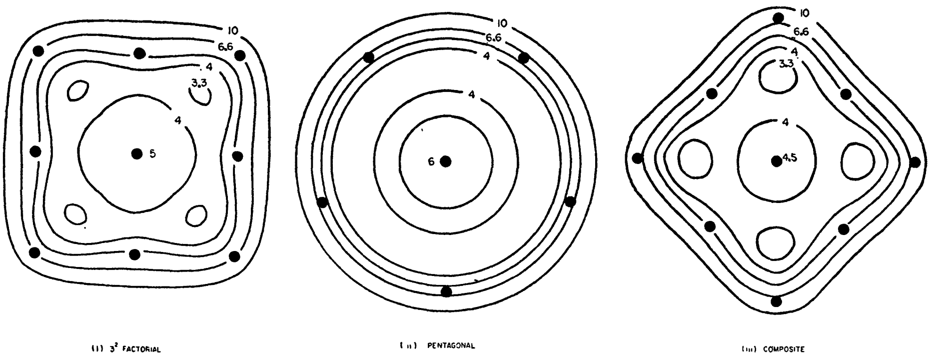

FIG. 2. Variance contours for some 2 dimensional designs

advance of the orientation of the surface relative to the design this also seems instinctively to be a sensible requirement for designs other than those of second order.

In general, for any $k-$ dimensional design, if the variance of the response estimated by the fitted polynomial is a function only of

$$\rho^2 = \sum_{i=1}^{k} x_i^2,$$

so that the variance contours in the space of the variables are circles, spheres or hyperspheres centered at the origin the design will be said to have a *spherical variance function* $V(\rho)$. An arrangement of points giving such a variance function will be called a rotatable design.

The remainder of this paper is devoted to constructing rotatable or nearly rotatable designs, that is, arrangements of experimental points which symmetrically generate information in those coordinates regarded as most relevant by the experimenter. We shall interpret requirement (a) in Section 1.3 in this sense.

5. Condition for rotatability. In the developments which follow we need some properties of derived power and product vectors and Schläflian matrices [7], [8], and [9]. If $\mathbf{x}' = (x_1, x_2, \cdots, x_k)$ then we denote by $\mathbf{x}'^{[p]}$ the derived power vector of degree p. For example if $k = 2$

$$\mathbf{x}' = [x_1, x_2] \qquad \text{and} \qquad \mathbf{x}'^{[2]} = [x_1^2, x_2^2, 2^{1/2}x_1 x_2]$$

and in general $\mathbf{x}'^{[p]}$ will contain as elements all the powers and products of total degree p and less (duly ordered) of the elements in $\mathbf{x}'$ with suitable multipliers attached so that $\mathbf{x}'^{[p]}\mathbf{x}^{[p]} = [\mathbf{x}'\mathbf{x}]^p$. If a vector $\mathbf{x}$ is transformed to a vector $\mathbf{z}$ by $\mathbf{z} = \mathbf{H}\mathbf{x}$, the pth Schläflian matrix $\mathbf{H}^{[p]}$ is defined such that $\mathbf{z}^{[p]} = \mathbf{H}^{[p]}\mathbf{x}^{[p]}$. It is readily confirmed that $[\mathbf{HK}]^{[p]} = \mathbf{H}^{[p]}\mathbf{K}^{[p]}$ and also that if $\mathbf{H}$ is orthogonal then so also is $\mathbf{H}^{[p]}$.

We need some properties of spherical distribution functions discussed in references [2], [10]. These distribution functions are of some importance in basic statistical theory, and especially in randomization theory, but these aspects are not pursued here.

5.1 *Moments of a spherical distribution.* If we have a set of random variables, $z_1, z_2, \cdots, z_k$, which may be regarded as the elements of a random vector $\mathbf{z}$, and each of which has zero mean and unit variance and if their joint distribution can be written in the form

$$p(\mathbf{z}) = kf(\mathbf{z}'\mathbf{z}), \qquad 0 \leqq \mathbf{z}'\mathbf{z} < W, \tag{16}$$

where W may be infinite and k is taken so that the integral over the whole space is unity, then since the density will be constant on hyper-spheres centered at the origin of the z's, we shall say that the variables have a spherical distribution.

Now if all the moments of a distribution exist, and the m.g.f. $\varphi(t)$ can be expanded in an infinite series, we can write this series

$$\varphi(\mathbf{t}) = 1 + \sum_{s=1}^{\infty} \frac{1}{s!} \mathbf{t}'^{[s]}\mathbf{m}_s, \tag{17}$$

where $\mathbf{m}_s$ is the vector of moments $\mathcal{E}\{\mathbf{z}^{[s]}\}$. But for a spherical distribution the moments are invariant under any orthogonal rotation of the coordinates whence the m.g.f. is

$$\varphi(\mathbf{t}) = \mathcal{E}(e^{\mathbf{t}'\mathbf{z}}) = \mathcal{E}(e^{\mathbf{t}'\mathbf{H}\mathbf{z}});$$

that is,

$$\varphi(\mathbf{t}) = \varphi(\mathbf{H}'\mathbf{t}) \tag{18}$$

for any orthogonal matrix $\mathbf{H}$. Regarding now the matrix $\mathbf{H}$ as transforming the matrix $\mathbf{t}'$, this implies that $\varphi(\mathbf{t})$ is unchanged by any transformation on $\mathbf{t}$ which leaves $\mathbf{t}'\mathbf{t}$ unchanged. The m.g.f. is therefore a function of $\mathbf{t}'\mathbf{t}$ and can be written in the form

$$\varphi(\mathbf{t}) = 1 + \sum_{p=1}^{\infty} \lambda_{2p} \frac{1}{p!2^p} (\mathbf{t}'\mathbf{t})^p, \tag{19}$$

where the λ's are real positive constants depending on the function f in (16). Equating terms in (17) and (19) and writing $[1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}]$ for the moment $\mathcal{E}[x_1^{\alpha_1}, x_2^{\alpha_2}, \cdots, x^{\alpha_k}]$ we have

$$[1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}] = \lambda_\alpha \frac{\prod_{i=1}^{k} \alpha_i!}{2^{\alpha/2} \prod_{i=1}^{k} (\frac{1}{2}\alpha_i)!}, \tag{20}$$

where $\alpha = \sum_{i=1}^{k} \alpha_i$ is called the order of the moment.

If the z's are independent so that

$$p(z) = \prod_{i=1}^{k} p(z_i), \tag{21}$$

then it has been shown, in references [11] and [12] that the only spherical distribution possible is the multi-variate normal with equal variances and zero covariances, which may be called the spherical multi-normal distribution. For this distribution the m.g.f. is

$$\varphi(t) = \exp[\tfrac{1}{2}(\mathbf{t}'\mathbf{t})] \tag{22}$$

and all the λ's are equal to unity. We see therefore that for any spherical distribution, the moments of the *same order* bear the same relationship to one another as do the moments for the spherical multi-normal. The moments of different orders will however depend on the λ's and hence on the function $f(\mathbf{z}'\mathbf{z})$.

5.2 *Variance of an estimated response.* Consider the response $\hat{y}_x$ estimated by a fitted polynomial of degree d at the point whose co-ordinates are given by the last k elements of the vector $\mathbf{x}'$ now defined as $\mathbf{x}' = (1, x_1, x_2, \cdots, x_k)$. The polynomial has $\binom{k+d}{d} = L$ terms and the estimated response at the point $x_1, x_2, \cdots, x_k$ is

$$\begin{aligned} \hat{y}_x = b_0 + b_1x_1 + b_2x_2 + \cdots + b_kx_k + b_{11}x_1^2 + b_{22}x_2^2 + \cdots \\ + b_{kk}x_k^2 + b_{12}x_1x_2 + \cdots + b_{k-1,k}x_{k-1}x_k + b_{111}x_1^3 + \text{etc.,} \end{aligned} \tag{23}$$

which may be written

$$\hat{y}_x = \mathbf{x}'^{[d]}\mathbf{b}, \tag{24}$$

where the $L \times 1$ vector $\mathbf{b}$ contains all the b's with suitable multipliers attached so that (24) is equivalent to (23). Suppose also that the true response at this point is given by

$$\eta_x = \mathbf{x}'^{[d]}\boldsymbol{\beta}. \tag{25}$$

Then for a given design matrix $\mathbf{D}$ for which there exists a matrix of independent variables $\mathbf{X}$ of full rank L the variance of $\hat{y}_x$ is

$$\begin{aligned} V(\hat{y}_x) = \mathcal{E}\{(\hat{y}_x - \eta_x)(\hat{y}_x - \eta_x)'\} = \mathbf{x}'^{[d]}\mathcal{E}\{(\mathbf{b} - \boldsymbol{\beta})(\mathbf{b} - \boldsymbol{\beta})'\}\mathbf{x}^{[d]} \\ = \mathbf{x}'^{[d]}[\mathbf{X}'\mathbf{X}]^{-1}\mathbf{x}^{[d]}\sigma^2. \end{aligned} \tag{26}$$

Consider now the variance of a second estimated value $\hat{y}_z$ which is the same distance ρ from the origin and whose co-ordinates are the last k elements of the vector $\mathbf{z} = \mathbf{R}\mathbf{x}$, where $\mathbf{R}$ is an orthogonal $(k + 1) \times (k + 1)$ matrix consisting of an arbitrary orthogonal matrix $\mathbf{H}$ bordered by a first row $\mathbf{u}' = (1, 0, 0, \cdots, 0)$ and a first column $\mathbf{u}$. Making the substitution in (26) we have

$$V(\hat{y}_z) = \mathbf{x}'^{[d]}\mathbf{R}'^{[d]}[\mathbf{X}'\mathbf{X}]^{-1}\mathbf{R}^{[d]}\mathbf{x}^{[d]}\sigma^2 \tag{27}$$

$$= \mathbf{x}'^{[d]}(\mathbf{R}'^{[d]}\mathbf{X}'\mathbf{X}\mathbf{R}^{[d]})^{-1}\mathbf{x}^{[d]}\sigma^2. \tag{28}$$

To satisfy the condition that the variance is constant on spheres centered at the origin of the design we require therefore that (28) and (26) are identically equal for every $\mathbf{x}$ and every $\mathbf{R}$. Whence

$$\mathbf{X'X} = \mathbf{R}'^{[d]}\mathbf{X'XR}^{[d]} \tag{29}$$

for every orthogonal matrix **R**. Now $N^{-1}\mathbf{R}'^{[d]}\mathbf{X'XR}^{[d]}$ is the moment matrix for the design matrix **HD**, and consequently the variance is constant for every point a distant ρ from the origin if and only if the moment matrix is invariant under orthogonal transformation of the design matrix. This means that unlike the 3^2 factorial design whose behavior under rotation is illustrated in Fig. 1, every variance and covariance of the b's and all the moments and mixed moments of the design must remain constant under rotation. We now need to find the form of moment matrix $N^{-1}\mathbf{X'X}$ for which Eq. (29) is satisfied.

5.3 *Moments of a rotable design.* We redefine the vector $\mathbf{t}'$ to be $(1, t_1, t_2, \cdots, t_k)$ and consider expression

$$Q = N^{-1}\mathbf{t}'^{[d]}\mathbf{X'Xt}^{[d]}, \tag{30}$$

which is a generating function for the moments of order $2d$ and less of the design. More specifically, since if $\mathbf{x}_u' = (1, x_{1u}, x_{2u}, \cdots, x_{ku})$, $\mathbf{X'X} = \sum_{u=1}^N \mathbf{x}_u^{[d]}\mathbf{x}_u'^{[d]}$, we have

$$\begin{aligned} Q &= N^{-1}\mathbf{t}'^{[d]}\left(\sum_{u=1}^{N} \mathbf{x}_u^{[d]}\mathbf{x}_u'^{[d]}\right)\mathbf{t}^{[d]} \\ &= N^{-1}\sum_{u=1}^{N} (\mathbf{t}'\mathbf{x}_u\mathbf{x}_u'\mathbf{t})^d \\ &= N^{-1}\sum_{u=1}^{N} (1 + t_1x_{1u} + t_2x_{2u} + \cdots + t_kx_{ku})^{2d}. \end{aligned} \tag{31}$$

Thus if we write $[1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}]$ for the moment $N^{-1}\sum_{u=1}^N x_{1u}^{\alpha_1} x_{2u}^{\alpha_2} \cdots x_{ku}^{\alpha_k}$ then the coefficient of $t_1^{\alpha_1}, t_2^{\alpha_2}, \cdots, t_k^{\alpha_k}$ in Q is

$$\frac{(2d)!}{\prod_{i=1}^{k} \alpha_i!(2d-\alpha)!}[1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}]. \tag{32}$$

Now from (29) the design is rotatable if and only if

$$Q = N^{-1}\mathbf{t}'^{[d]}\mathbf{X'Xt}^{[d]} \equiv N^{-1}\mathbf{t}'^{[d]}\mathbf{R}'^{[d]}\mathbf{X'XR}^{[d]}\mathbf{t}^{[d]} \tag{33}$$

$$= N^{-1}(\mathbf{t'R'})^{[d]}\mathbf{X'X}(\mathbf{Rt})^{[d]}; \tag{34}$$

that is to say, if any transformation which leaves $\mathbf{t't}$ unchanged does not change Q. Hence the design is rotatable if and only if Q is some function of $\mathbf{t't}$ and since it is a polynomial in the t's it must be of the form

$$Q = \sum_{s=0}^{d} a_{2s}\left(\sum_{i=1}^{k} t_i^2\right)^s. \tag{35}$$

The coefficient of $t_1^{\alpha_1}, t_2^{\alpha_2}, \cdots, t_k^{\alpha_k}$ in this expression is zero if any of the α_i are odd integers. If the α_i are even integers the coefficient is

$$a_\alpha(\tfrac{1}{2}\alpha)! \Big/ \prod_{i=1}^{k} (\tfrac{1}{2}\alpha_i)!. \tag{36}$$

We may now equate coefficients to obtain specific values for the moments to order $\alpha = 2d$ as follows

$$[1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}] = \frac{a_\alpha(\frac{1}{2}\alpha)!(2d - \alpha)!}{2d!} \cdot \frac{\prod_{i=1}^{k} \alpha_i!}{\prod_{i=1}^{k} (\frac{1}{2}\alpha_i)!}; \tag{37}$$

and if we write

$$\frac{a_\alpha 2^{\alpha/2}(\frac{1}{2}\alpha)!(2d - \alpha)!}{2d!} = \lambda_\alpha, \tag{38}$$

then finally the moments of a rotatable design of order d are

$$\begin{aligned} [1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}] &= 0 && \text{if one or more of the } \alpha_i \text{ are odd,} \\ &= \lambda_\alpha \frac{\prod_{i=1}^{k} \alpha_i!}{2^{\alpha/2} \prod_{i=1}^{k} (\frac{1}{2}\alpha_i)!} && \text{if all of the } \alpha_i \text{ are even,} \end{aligned} \tag{39}$$

which are the moments up to order $2d$ of a spherical distribution.

5.4 *Effect of transformations on zero moments.* It is readily seen that if the original variables $x_1, x_2, \cdots, x_k$ are transformed by any non-singular linear transformation to variables $X_1, X_2, \cdots, X_k$ then any moment of order α for the new variables will be a linear combination of moments all of order α for the old variables. It follows in particular that if an arrangement of points is such that *all* the moments of a given odd order are zero then they remain zero in every orientation of the arrangement.

6. Moment requirements for rotatable designs of first and second order. It has been shown that the moment matrix for a rotatable design of order d has a specific form which is invariant under orthogonal rotation of the axes of the variables. The moments which are the elements of this moment matrix are the same as those of a spherical distribution and are known apart from arbitrary constants $\lambda_0, \lambda_2, \cdots, \lambda_{2d}$. The variance function $V(\rho)$ for a rotatable design depends only on $\lambda_0, \lambda_2, \cdots, \lambda_{2d}$ and on $\rho = (\mathbf{x}'\mathbf{x})^{1/2}$. In selecting a design of order d we can proceed as follows:

(a) Using Eq. (39) we first obtain in terms of the λ's the form of the moment matrix for a rotatable design of the required order.

(b) Since for a rotatable design the variance function depends, apart from the λ's, only on ρ it is now comparatively easy to study the effect on the variance function of varying the λ's. Having selected the λ's to give a satisfactory variance function and alias matrix the required form of the moment matrix is completely defined.

(c) We have then to determine actual arrangements of points which, so far as possible, satisfy the requirements listed in Section 1.3 as well as these moment conditions.

From Eq. (39), $\lambda_0 = [0]$ and $\lambda_2 = [ii]$, $(i = 1, 2, \cdots, k)$. Since by convention $[0] = [ii] = 1$, λ_0 and λ_2 are always equal to unity, and no element of choice for the λ's arises with rotatable designs of first order, but only with designs of order 2, 3, etc., for which the values of λ_4, λ_6, etc., must be selected. In making this selection both the variance function and the alias matrix must be considered. It will be recalled that the alias matrix contains as elements the coefficients of biases which arise in the estimated coefficients when the assumed form of the model is inadequate. For a design of order d it is natural to first consider biases arising from terms of order $d + 1$ not allowed for in the assumed form of the model. If we suppose that the true form of the model is of order $d + 1$ it will be clear from the form of the alias matrix $\mathbf{A}$ in Eq. (8a) that for a rotatable design of order d the coefficients of the biases can be completely expressed in terms of $\lambda_0, \lambda_2, \cdots, \lambda_{2d}$ and the moments of order $2d + 1$. When possible, it is advantageous to use a rotatable design of order d for which all moments of order $2d + 1$ are zero. From Section 5.4 these moments are then zero in every orientation. The alias matrix $\mathbf{A}$ is a function only of the λ's and all biases arising from terms of order $d + 1$ are avoided except those which arise inevitably because the bias coefficients are functions of the λ's themselves.

The remainder of the present section is devoted to determining the necessary form of the moment matrix and to discussing the properties of designs of first and second order. Specific second order designs having the required form of moment matrix are derived in Section 7.

6.1 *Rotatable designs of order* 1. Suppose we have k variables $x_1, x_2, \cdots, x_k$ and we desire to fit a polynomial of degree $d = 1$, that is to say, a fitted equation representing a plane

$$\hat{y}_x = b_0 + b_1x_1 + b_2x_2 + \cdots + b_kx_k. \tag{40}$$

Then from Eq. (39), for a k-dimensional rotatable design of first order

all moments $[i]$ $(i = 1, 2, \cdots, k)$ of order 1 are zero,

mixed moments $[ij]$ $(i \neq j = 1, 2, \cdots, k)$ of order 2 are zero,

quadratic moments $[ii]$ $(i = 1, 2, \cdots, k)$ of order 2 $= \lambda_2 = 1$.

Thus the moment matrix $N^{-1}\mathbf{X}'\mathbf{X}$ is $\mathbf{I}_{k+1}$.

The condition that a first order design is rotatable is thus precisely the same as that it should have smallest variances, namely that its moment matrix should be the identity matrix.

The variance function for this type of design is given by

$$NV(\hat{y}_x)/\sigma^2 = V(\rho) = (1 + \rho^2), \tag{41}$$

where $\rho = \left\{ \sum_{i=1}^{k} x_i^2 \right\}^{1/2}$.

The standardized weight function $W(\rho) = [V(\rho)]^{-1}$, which shows the relative precision of the estimate $\hat{y}$ at a distance ρ from the center of the design, for any first order rotatable design is graphed in Fig. 3.

Setting aside our scaling convention we see that in general the variance of

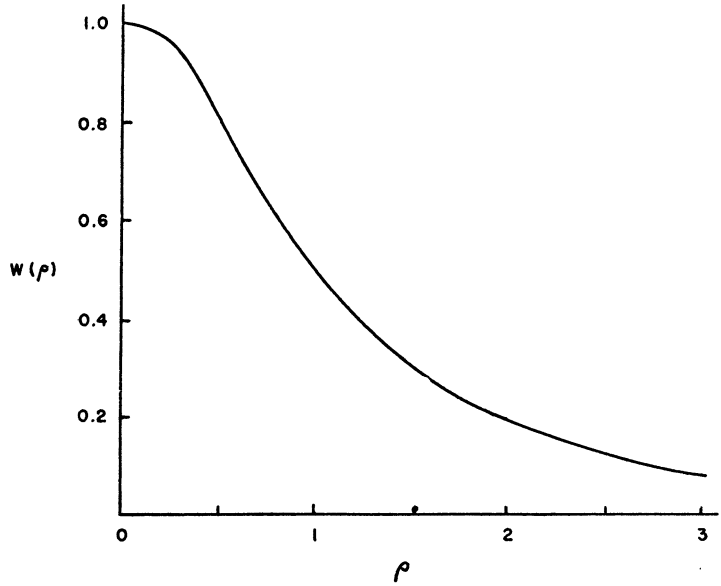

FIG. 3. Weight function for any first order rotatable design

the estimated response at a distance ρ from the center of any rotatable design of first order is given simply by

$$V(\hat{y}) = V(b_0) + V(b_i)\rho^2. \tag{41a}$$

This is of the same form as the well-known formula for a single variable x with ρ replacing x.

6.11. *Biases due to second order coefficients.* If it happens, contrary to assumption, that terms of second order are not negligible, then using Eq. 8a, the expected values of the estimated coefficients for any first order rotatable design are as follows

$$\begin{aligned} \mathcal{E}(b_0) &= \boldsymbol{\beta}_0 + \boldsymbol{\lambda}_2 \sum_{g=1}^{k} \boldsymbol{\beta}_{gg} \\ \mathcal{E}(b_i) &= \boldsymbol{\beta}_i + \sum_{g=1}^{k} \sum_{h=g}^{k} [ghi]\beta_{gh}. \qquad (i = 1, 2, \cdots, k) \end{aligned} \tag{42}$$

Those terms printed in boldface type inevitably arise but those in ordinary type may be eliminated by a suitable choice of the design. On our convention λ_2 is equal to unity and it follows that, if β_0 is estimated assuming a first order model, then when the quadratic coefficients β_{gg} are not zero, bias in this estimate is inevitable. In general the coefficients $[ghi]$ of the biases in the estimates of the linear coefficients β_i will vary as the design is rotated (see reference [2] for particular examples of this). By selecting a design for which all the third order moments are zero we may eliminate bias in the estimates of the linear coefficients in every orientation of the design (see Section 5.4). Specific designs of this sort were discussed in [1] under the name "first order designs of type B." They can be obtained by duplicating with reversed signs any orthogonal first order design, in particular any of the "simplex" designs of [2], [5]. The two-level factorial designs and many of the fractional factorials are also examples of particular orientations of designs of this sort.

6.2. *Rotatable designs of order two.* Suppose we have k variables, and desire to fit a polynomial of degree two. From (39) the moments of a k-dimensional second order rotatable design suitable for this situation are such that all odd moments are zero, and the remaining moments are $[ii] = \lambda_2 = 1$, $[iijj] = \lambda_4$, $[iiii] = 3\lambda_4$.

Thus for a second order rotatable design the moment matrix is of the form:

$$
(43) \qquad N^{-1}\mathbf{X}'\mathbf{X} =
\begin{array}{r}
 \\ 0 \\ 1 \\ 2 \\ \cdot \\ \cdot \\ \cdot \\ k \\ 11 \\ 22 \\ \cdot \\ \cdot \\ \cdot \\ kk \\ 12 \\ 13 \\ \cdot \\ \cdot \\ \cdot \\ k-1,k
\end{array}
\left[\begin{array}{c|cccccc|ccccc|ccccc}
0 & 1 & 2 & \cdots & & & k & 11 & 22 & \cdots & & kk & 12 & 13 & \cdots & & k-1,k \\
1 & & & * & & & & 1 & 1 & \cdots & & 1 & & & * & & \\
\hline
 & 1 & & & & & & & & & & & & & & & \\
 & & 1 & & & & & & & & & & & & & & \\
* & & & \cdot & & & & & & * & & & & & * & & \\
 & & & & \cdot & & & & & & & & & & & & \\
 & & & & & \cdot & & & & & & & & & & & \\
 & & & & & & 1 & & & & & & & & & & \\
\hline
1 & & & & & & & 3\lambda_4 & \lambda_4 & \cdots & & \lambda_4 & & & & & \\
1 & & & & & & & \lambda_4 & 3\lambda_4 & \cdots & & \lambda_4 & & & & & \\
\cdot & & & * & & & & \cdot & \cdot & & & \cdot & & & * & & \\
\cdot & & & & & & & \cdot & \cdot & & & \cdot & & & & & \\
\cdot & & & & & & & \cdot & \cdot & & & \cdot & & & & & \\
1 & & & & & & & \lambda_4 & \lambda_4 & \cdots & & 3\lambda_4 & & & & & \\
\hline
 & & & & & & & & & & & & \lambda_4 & & & & \\
 & & & & & & & & & & & & & \lambda_4 & & & \\
* & & & * & & & & & & * & & & & & \cdot & & \\
 & & & & & & & & & & & & & & & \cdot & \\
 & & & & & & & & & & & & & & & & \cdot \\
 & & & & & & & & & & & & & & & & \lambda_4
\end{array}\right]
$$

where the asterisks indicate null submatrices.

The inverse matrix (i.e. the precision matrix) is readily shown to be

$$
(44) \qquad N(\mathbf{X}'\mathbf{X})^{-1} =
\begin{array}{r}
 \\ 0 \\ 1 \\ 2 \\ \cdot \\ \cdot \\ k \\ 11 \\ 22 \\ \cdot \\ \cdot \\ \cdot \\ kk \\ 12 \\ 13 \\ \cdot \\ \cdot \\ k-1,k
\end{array}
\left[\begin{array}{c|ccccc|cccc|cccc}
0 & 1 & 2 & \cdots & & k & 11 & 22 & \cdots & kk & 12 & 13 & \cdots & k-1,k \\
2\lambda_4^2(k+2)A & & & * & & & -2\lambda_4 A & -2\lambda_4 A & \cdots & -2\lambda_4 A & & & * & \\
\hline
 & 1 & & & & & & & & & & & & \\
 & & 1 & & & & & & & & & & & \\
* & & & \cdot & & & & * & & & & & * & \\
 & & & & \cdot & & & & & & & & & \\
 & & & & & 1 & & & & & & & & \\
\hline
-2\lambda_4 A & & & & & & [(k+1)\lambda_4-(k-1)]A & (1-\lambda_4)A & \cdots & (1-\lambda_4)A & & & & \\
-2\lambda_4 A & & & & & & (1-\lambda_4)A & [(k+1)\lambda_4-(k-1)]A & \cdots & (1-\lambda_4)A & & & & \\
\cdot & & & * & & & \cdot & \cdot & & \cdot & & & * & \\
\cdot & & & & & & \cdot & \cdot & & \cdot & & & & \\
\cdot & & & & & & \cdot & \cdot & & \cdot & & & & \\
-2\lambda_4 A & & & & & & (1-\lambda_4)A & (1-\lambda_4)A & \cdots & [(k+1)\lambda_4-(k-1)]A & & & & \\
\hline
 & & & & & & & & & & \lambda_4^{-1} & & & \\
 & & & & & & & & & & & \lambda_4^{-1} & & \\
* & & & * & & & & * & & & & & \cdot & \\
 & & & & & & & & & & & & & \cdot \\
 & & & & & & & & & & & & & \lambda_4^{-1}
\end{array}\right]
$$

where

$$A = [2\lambda_4\{(k + 2)\lambda_4 - k\}]^{-1}. \tag{45}$$

The variances and covariances of the estimated coefficients using any second order rotatable design are therefore given by

$$\begin{aligned} &\frac{NV(b_0)}{\sigma^2} = 2\lambda_4^2(k + 2)A; \quad \frac{NV(b_i)}{\sigma^2} = 1; \\ &\frac{NV(b_{ii})}{\sigma^2} = [(k + 1)\lambda_4 - (k - 1)]A; \quad \frac{NV(b_{ij})}{\sigma^2} = \lambda_4^{-1}; \\ &\frac{N \operatorname{Cov}(b_0, b_{ii})}{\sigma^2} = -2\lambda_4 A; \quad \frac{N \operatorname{Cov}(b_{ii} b_{jj})}{\sigma^2} = (1 - \lambda_4)A \end{aligned} \tag{46}$$

and all the remaining covariances are zero. Thus all first and second degree coefficients are uncorrelated except the quadratic coefficients. These have a coefficient of correlation $\{[2/(1 - \lambda_4)] - (k + 1)\}^{-1}$.

If we put $\lambda_4 = 1$ the correlations between the quadratic coefficients are all zero and the design is orthogonal (in the sense of Section 3) as well as rotatable. We then have

$$\begin{aligned} &\frac{NV(b_0)}{\tau^2} = \tfrac{1}{2}(k + 2); \quad \frac{NV(b_i)}{\sigma^2} = 1; \quad \frac{NV(b_{ii})}{\sigma^2} = \tfrac{1}{2}; \\ &\frac{NV(b_{ij})}{\sigma^2} = 1; \quad \frac{N \operatorname{Cov}(b_0 b_{ij})}{\sigma} = -\tfrac{1}{2}. \end{aligned} \tag{47}$$

The conditions of rotatability and orthogonality together fix the relative variances for effects of different orders. In particular for designs of this sort the variances of the quadratic coefficients b_{ii} are one half those of the two-factor interaction coefficients b_{ij}, in contrast with three-level factorial designs for which the variances of the quadratic coefficients are twice those for the interaction coefficients. Compared with the factorial in standard orientation, the orthogonal rotatable design thus places four times as much emphasis on the quadratic coefficient relative to the interaction coefficients. From (44) the variance function for any general second order rotatable design is given by

$$V(\rho) = A\{2(k + 2)\lambda_4^2 + 2\lambda_4(\lambda_4 - 1)(k + 2)\rho^2 + [(k + 1)\lambda_4 - (k - 1)]\rho^4\}, \tag{48}$$

and for the particular case of orthogonal second order rotatable design by

$$V(\rho) = \tfrac{1}{2}(k + 2 + \rho^4). \tag{48a}$$

Setting aside for the moment our scaling convention we see that in general the variances of the estimated response at a distance ρ from the center of any rotatable second order design is simply given by

$$V(\hat{y}) = V(b_0) + 2 \operatorname{Cov}(b_0 b_{ii})\rho^2 + V(b_i)\rho^2 + V(b_{ii})\rho^4.$$

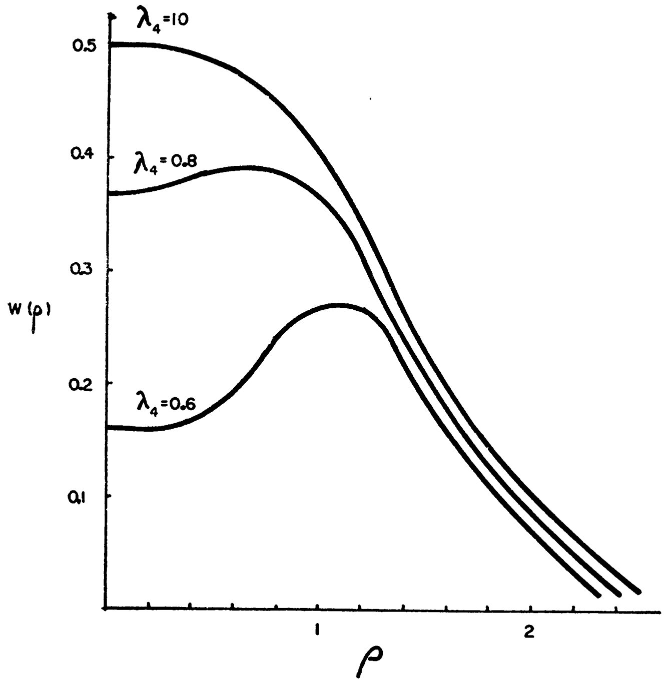

FIG. 4. Weight functions for second order rotatable designs having various values of λ when $k = 2$

This, with ρ replacing x, is of the form obtained for a single variable x when the design employed is any symmetric arrangement.

In Fig. 4 the standardized weight function $W(\rho) = \{V(\rho)\}^{-1}$ is graphed for various values of λ_4 for the case of a two dimensional second order design. Similar graphs are obtained for other values of k.

We notice that whatever value of λ_4 is chosen the precision falls off rapidly when ρ exceeds unity. If we chose $\lambda_4 = 1$ the design is orthogonal in the sense discussed previously. When λ_4 approaches or exceeds unity, the precision, particularly at the center of the design, is high but the bias coefficients are high also. It is well to remember at this point that we are comparing designs for which the "spread" of points, as measured by the marginal second moments $S_i^2 = N^{-1}\sum_{u=1}^{N} (\xi_{iu}^2 - \bar{\xi}_i)^2$, is constant. Such a convention is bound to favor designs with a high value of λ_4, so that although the general shape of the design weight function will be meaningful, the absolute height of the curve at any point will be to some extent an outcome of this convention. It seems reasonable to seek a relatively uniform distribution of precision in the immediate vicinity of the design. This is attained with a value of λ_4 somewhat less than unity and such a choice will give satisfactory values for the third order bias coefficient. In particular, if the variance at $\rho = 1$ is to equal the variance at $\rho = 0$, the values of λ_4 shown in Table 1 will be needed.

TABLE 1

Values of λ_4 required to make the variance at $\rho = 1$ equal to that at $\rho = 0$

k	2	3	4	5	6	7	8
λ_4	0.7844	0.8385	0.8704	0.8918	0.9070	0.9184	0.9274

So far we have supposed that our interest centers on the absolute value of η as estimated by $\hat{y}$. In some circumstances we would be more interested in the relative value of η rather than in its absolute magnitude. For example, the estimation of the slope of a first degree surface, or of the position of the stationary point on a fitted second degree surface, does not require knowledge of the absolute value of η but only of its value at one point in the space of the variables relative to its value at some other point.

A natural reference value is β_0, the response at the origin of the design, and he appropriate estimate of

$$\Delta = \eta - \beta_0 = \beta_1 x_1 + \cdots + \beta_k x_k + \beta_{11} x_1^2 + \text{etc.}$$

is

$$\hat{d} = b_1 x_1 + \cdots + b_k x_k + b_{11} x_1^2 + \text{etc.}$$

For the rotatable designs already discussed, $V(\hat{d})$ as well as $V(\hat{y})$ is constant at a constant distance ρ from the center of the design. At a point distance ρ from the center, for any first order rotatable design, we have simply

$$V(\hat{d}) = V(b_i)\rho^2 \tag{49}$$

and for any second order rotatable design

$$V(\hat{d}) = V(b_i)\rho^2 + V(b_{ii})\rho^4. \tag{49a}$$

It is not our intention at this time to claim optimal properties for the designs which are here derived. The only justification presented is that these arrangements symmetrically generate information in the coordinates regarded as most relevant by the experimenter. An approach which makes it possible to measure the practical efficiency of these and other arrangements has however been attempted and it is hoped to publish this elsewhere. In this more complete appraisal of the situation, a citerion on the effectiveness of the design is taken as the integrated mean square error of $\hat{y}$ over the region of interest to the experimenter. The scale of the design, and the constants such as λ_4, which reflect the distribution of the experimental points, are so chosen as to minimize this criterion. The integrated mean square error contains two terms: one which measures the variance of $\hat{y}$ and the other the bias in $\hat{y}$ due to possible inadequacies of the assumed model. As λ_4 is increased the variance term becomes smaller and the bias term becomes larger. The problem is to strike some compromise which will be satisfactory for practical situations. It appears that the values of λ_4 given in Table 1, although perfectly satisfactory, may be a little high in the light of this more recent work.

In the present paper we consider the nature of the bias in the estimates of the individual coefficients rather than the nature of the bias in $\hat{y}$.

6.21. *Biases due to third order constants.* If it happens, contrary to assumption, that terms of third order are not negligible, then using equation 8(a), the expected values of the estimated constants for any second order rotatable design are as follows:

$$\mathcal{E}(b_0) = \boldsymbol{\beta}_0 - 2\lambda_4 A \sum_{f=1}^{k} \sum_{g=f}^{k} \sum_{h=g}^{k} \sum_{i=1}^{k} [fghii]\beta_{fgh}\,, \tag{50}$$

$$\mathcal{E}(b_i) = \boldsymbol{\beta}_i + 3\lambda_4 \boldsymbol{\beta}_{iii} + \lambda_4 \sum_{h \neq i}^{k} \boldsymbol{\beta}_{hhi}\,, \tag{51}$$

$$\begin{aligned}\mathcal{E}(b_{ii}) = \boldsymbol{\beta}_{ii} + \{(k+2)\lambda_4 - k\}A[iiiii]\beta_{iii} \\ + (1-\lambda_4)A \sum_{f=1}^{k} \sum_{g=f}^{k} \sum_{h=g}^{k} \sum_{i=1}^{k} [fghii]\beta_{fgh}\,,\end{aligned} \tag{52}$$

$$\mathcal{E}(b_{ij}) = \boldsymbol{\beta}_{ij} + \lambda_4^{-1} \sum_{f=1}^{k} \sum_{g=f}^{k} \sum_{h=g}^{k} [fghij]\, \beta_{fgh}\,. \tag{53}$$

Again terms printed in boldface type arise inevitably but those in ordinary type may be eliminated in every orientation by selecting a design for which all the fifth order moments are zero.

The requirements and properties of rotatable designs of third and higher order may be studied in the same way as for designs of order 1 and 2. We shall not pursue this topic here but will now consider how we may obtain actual arrangements of points which satisfy the requirements for rotatable designs of second order.

7. Examples of second order rotatable designs. The above discussion has been directed to deciding what type of design we should be seeking. We have shown the moment conditions which a design of any given order must satisfy to obtain constant precision on spheres centered at the origin of the design. We now consider the problem of finding arrangements of experimental points which satisfy these conditions. The classes of rotatable designs we discuss are by no means exhaustive but rather are intended to illustrate some of the possibilities.

We mention in passing that for any design of order d which is both orthogonal in the sense already discussed, and rotatable, has moments up to order $2d$ which are the same as those of the spherical multinormal distribution. This is of interest since it shows that in the usual multiple regression problem where the values of the independent variables $x_1, x_2, \cdots, x_k$ are not held at predetermined levels but are allowed to vary at random we should obtain a good arrangement, if it happened the x's followed a multivariate normal distribution with zero covariances—a conclusion which is intuitively very acceptable. Rotatable designs could be approximated simply by taking independent random samples from a normal distribution, but in fact it is possible to satisfy the criterion of rotatability exactly.

We have seen that for a rotatable design of order d the moments must be the same up to order $2d$ as those of a spherical density function. This suggests that we might construct rotatable designs by equally spacing the available finite number of experimental points on one or more spheres.

We find in fact that it is convenient to regard designs as built up from a number of component sets of points each set having its points all equidistant from the origin. This we call an equiradial set and ρ the distance of each point from the origin the radius of the set. If the moments to order $2d$ of such a set are unchanged by rotation we call this an equiradial rotatable set of order d.

An equiradial rotatable set of order d does not necessarily, or even usually, of itself provide a design. For example, n points at the origin provide an equiradial set of infinite order. Furthermore, no single equiradial set can provide a design of order greater than one, for if ρ is the common distance from the origin then

$$\sum_{i=1}^{k} x_{iu}^2 = \rho^2 x_{0u}, \qquad u = 1, 2, \cdots, N.$$

It follows that if $d > 1$ the matrix of independent variables for such an arrangement is singular and the quadratic coefficients $b_{11}, b_{22}, \cdots, b_{kk}$ and the constant term b_0 cannot be separately estimated.

As is shown later we can obtain equiradial sets of points which satisfy the moment conditions (39) for rotatable design of order 2 but only for such values of λ_4 as lead to a singular moment matrix. For such a set of points $\rho^2 = \sum_{i=1}^{k} x_{iu}^2$ for $u = 1, 2, \cdots, N$, whence

$$\rho^2 = N^{-1} \sum_{u=1}^{N} \sum_{i=1}^{k} x_{iu}^2 = \sum_{i=1}^{k} [ii] = k; \tag{54}$$

also,

$$\rho^4 = N^{-1} \sum_{u=1}^{N} \left\{ \sum_{i=1}^{k} x_{iu}^2 \right\}^2 = \sum_{i=1}^{k} [iiii] + \sum_{i=1}^{k} \sum_{j \neq i}^{k} [iijj], \tag{55}$$

whence

$$3k\lambda_4 + k(k-1)\lambda_4 = k^2 \tag{56}$$

and

$$\lambda_4 = k/(k+2). \tag{57}$$

When this value of λ_4 is substituted in (45) and (46) the quantity A becomes infinite and the quadratic terms and the constant term are not separately estimable. We shall refer to this value λ_4 as the "singular" value.

Now although no single equiradial set can supply a usable second order design, two or more sets can do so. Suppose we have s equiradial rotatable sets of points having the same origin such that in the wth set there are n_w points each at a distance ρ_w from the origin then the value of λ_4 for the whole aggregate of the $N = \sum_{w=1}^{s} n_w$ points is

$$(58) \qquad \lambda_4 = \frac{Nk \sum_{w=1}^{s} n_w \rho_w^4}{(k+2)\left(\sum_{w=1}^{s} n_w \rho_w^2\right)^2},$$

which will not in general have a singular value. By combining equiradial sets we can thus obtain rotatable designs. Since a set of points at the origin will affect only the value of N in (58) the formula may be applied without modification to designs for which one set of points is at the center. In practice, we shall find that the placing of one or more points at the center of an equiradial rotatable set provides one useful means of modifying the value of λ_4. If there are n_1 points at the origin and n_2 points in the equiradial rotatable set we see that for the aggregate of $n_1 + n_2$ points

$$(59) \qquad \lambda_4 = \frac{k(n_1 + n_2)}{(k+2)n_2}.$$

We now show that sets of points which are equally spaced on a circle, a sphere, or a hypersphere and which thus form the vertices of a regular polygon, polyhedron, or polytope, can provide rotatable sets which may be combined to form rotatable designs. Our study begins with the two dimensional figures.

7.1 *Two dimensional designs.* We first show that for the vertices of a regular n-gon, all moments up to order $n - 1$ are invarient under rotation.

Suppose the coordinates of the uth point are $\rho \cos(\varphi + 2\pi u/n)$ and $\rho \sin(\varphi + 2\pi u/n)$ and that $a = e^{i\varphi}$ and $\omega = e^{i2\pi/n}$. We have for the moment $[pq]$ which is of order $p + q$

$$(60) \qquad [pq]_\varphi = (\tfrac{1}{2}\rho)^{p+q} i^{-q} \sum_{u=0}^{n-1} (a\omega^u + a^{-1}\omega^{-u})^p (a\omega^u - a^{-1}\omega^{-u})^q.$$

After expanding the bracketed expressions and collecting terms

$$(61) \qquad [pq]_\varphi = (\tfrac{1}{2}\rho)^{p+q} \sum_{r=0}^{p} \sum_{t=0}^{q} i^{2t-q} \binom{p}{r}\binom{q}{t} a^{p+q-2(r+t)} \sum_{u=0}^{n-1} \omega^{u\{p+q-2(r+t)\}}.$$

By putting $a = 1$ in the expression and substituting the result from (61) we obtain the change in the value of the moment after rotation through an angle φ:

$$(62) \quad [pq]_\varphi - [pq]_0 = (\tfrac{1}{2}\rho)^{p+q} \sum_{r=0}^{p} \sum_{t=0}^{q} i^{2t-q} \binom{p}{r}\binom{q}{t} [a^{p+q-2(r+t)} - 1] \sum_{u=0}^{n-1} \omega^{u\{p+q-2(r+t)\}}.$$

Now

$$(63) \qquad \sum_{u=0}^{n-1} \omega^{u\{p+q-2(r+t)\}} \begin{aligned} &= n \quad \text{if } p + q - 2(r+t) = 0 \text{ or } mn \text{ where } m \text{ is an integer,} \\ &= 0 \quad \text{otherwise,} \end{aligned}$$

and $-(p+q) \leqq p+q-2(r+t) \leqq p+q$. Thus if $(p+q) < n$ the expression on the left of (63) is zero unless $p+q = 2(r+t)$, but in this case a $a^{\{p+q-2(r+t)\}} - 1 = 0$. Hence if $p+q < n$ then (62) is zero whatever the value of φ and our assertion is proved.

A class of two-dimensional second order rotatable designs may be constructed therefore from two or more concentric rings of equispaced points with unequal radii. Points at the origin constitute a ring of zero radius and each ring which is not of zero radius must contain at least five points. The number of the points in each set and the radial distances will determine the value of λ_4 in accordance with equation (58).

Of this class of designs the simplest are those having one ring of $n_2 \geqq 5$ equally spaced points with additional n_1 points at the origin.

Pentagonal designs with center points. Putting $n_2 = 5$ we obtain the following values of λ_4 for specimen numbers of center points

Number of points at center of pentagon............	1	3	5
Value of λ_4..................................	0.6	0.8	1.0

By using three points at the center a value of $\lambda_4 = 0.8$ is obtained which is close to that given in Table 1. For orthogonality five center points are required.

Hexagonal designs with center points. If we put n_2 equal to six so that the external points are at the vertices of a hexagon, we obtain the added advantage that all the moments of order 5 are zero thus insuring that in every orientation of the design the estimate b_0 and the estimates b_{ii}, b_{ij} of the second order coefficients are not biased by any third order terms. A value of λ_4 close to that given in Table 1 is obtained by placing $n_1 = 3$ points at the center. "Orthogonality" is obtained when $n_1 = 6$.

Designs containing two rings of points. A variety of designs, which however use more than ten points, can be obtained by combining two or more concentric circles of equispaced points. Table 2, below, shows some of the alternatives. Values of the ratio of radii are shown (i) which give $\lambda_4 = 0.7844$, the value given in Table 1, and (ii) which give $\lambda_4 = 1.0$, the value required for orthogonality.

TABLE 2

Radii for equispaced points on concentric circles

n_1	5	5	5	6	6	7
n_2	6	7	8	7	8	8
ρ_2/ρ_1 for $\lambda_4 = 0.7844$	0.414	0.438	0.454	0.407	0.430	0.404
ρ_2/ρ_1 for $\lambda_4 = 1.0$	0.204	0.267	0.304	0.189	0.250	0.176

The arrangements so far discussed by no means exhaust the possible second order designs in two dimensions. A further class of designs is obtained by combining sets of equiradial points which are not individual rotatable sets of order 2. For example, sets of three points each of which form the vertices of an equilateral triangle with center coincident with the origin, may be combined to form such arrangements. Suppose that a line, assumed to be of length $\rho\sqrt{2}$ and connecting one of the vertices of an equilateral triangle to the center makes an angle φ with the x_2 axis. Then it is easily shown that the second order moment matrix for this arrangement is

$$N^{-1}\mathbf{X}'\mathbf{X} = \begin{array}{c} \\ \\ \end{array}\begin{matrix} 0 & 1 & 2 & 11 & 22 & 12 \end{matrix}$$

$$N^{-1}\mathbf{X}'\mathbf{X} = \begin{bmatrix} 1 & \cdot & \cdot & \rho^2 & \rho^2 & \cdot \\ \cdot & \rho^2 & \cdot & \rho^3 a & -\rho^3 a & -\rho^3 b \\ \cdot & \cdot & \rho^2 & -\rho^3 b & \rho^3 b & -\rho^3 a \\ \rho^2 & \rho^3 a & -\rho^3 b & \frac{3}{2}\rho^4 & \frac{1}{2}\rho^4 & \cdot \\ \rho^2 & -\rho^3 a & \rho^3 b & \frac{1}{2}\rho^4 & \frac{3}{2}\rho^4 & \cdot \\ \cdot & -\rho^3 b & -\rho^3 a & \cdot & \cdot & \frac{1}{2}\rho^4 \end{bmatrix},$$

where $a = 2^{-\frac{1}{2}} \sin 3\varphi$ and $b = 2^{-\frac{1}{2}} \cos 3\varphi$.

This is of the form required for rotatability except for the elements containing a and b. Suppose s arrangements of this sort are combined, the wth such arrangement having $\rho = \rho_w$ and $\varphi = \varphi_w$. Then the moment matrix will be of the exact form required for rotatability if

(64) $$\sum_{w=1}^{s} \rho_w^3 \sin 3\varphi_w = 0 \quad \text{and} \quad \sum_{w=1}^{s} \rho_w^3 \cos 3\varphi_w = 0.$$

This implies simply that the sum of the s vectors

$$(\rho_1^3 \cos 3\varphi_1,\ \rho_1^3 \sin 3\varphi_1),\ \cdots,\ (\rho_s^3 \cos 3\varphi_s,\ \rho_s^3 \sin 3\varphi_s)$$

shall be zero (i.e., they form the sides of some polygon) and an infinity of solutions is at once obtainable.

The value of λ_4 for such a design is

(65) $$\lambda_4 = \tfrac{1}{2}s \sum_{w=1}^{s} \rho_w^4 \Big/ \left(\sum_{w=1}^{s} \rho_w^2\right)^2.$$

If $s = 2$, then to satisfy (64) the two vectors must be of the form

$$(\rho^3 \cos 3\varphi,\ \rho^3 \sin 3\varphi) \quad \text{and} \quad (-\rho^3 \cos 3\varphi,\ -\rho^3 \sin 3\varphi),$$

where φ is arbitrary. The design then consists of the vertices of a hexagon with λ_4 equal to its singular value.

If $s > 2$ an infinite variety of these designs, in which the sets of points have different radii and appropriate relative orientations, can be derived. The largest value of λ_4 is obtained when all but two of the ρ_w are zero. The two non-zero vectors are equal in magnitude and opposite in sign and $\lambda_4 = \frac{1}{4}s$. The resulting design then consists of the vertices of a hexagon in any orientation together with the remaining $3(s - 2)$ points at the center.

Designs may similarly be built up from combinations of regular figures having

2 and 4 points. As before the maximum value of λ_4 is obtained by having a single ring of equispaced points plus points at the center.

7.2 *Rotation of Set of Points in k dimensional space.* In order to investigate the possibilities in more than two dimensions we first consider a method for studying the effect on the moment matrix of rotating any k-dimensional arrangement of experimental points.

Consider some set of N points in k dimensional space and as before denote by $\mathbf{D}$ the $N \times k$ design matrix, the elements of whose rows are the coordinates of the points. To correspond to our definition of derived power vectors suppose a second degree model written so that product terms such as $x_i x_j$ have the coefficient $\sqrt{2}$ attached. For example, if $k = 3$

$$(66)\qquad \begin{aligned} \eta = {} & \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 \\ & + \frac{\beta_{12}}{\sqrt{2}} (\sqrt{2}\, x_1 x_2) + \frac{\beta_{13}}{\sqrt{2}} (\sqrt{2}\, x_1 x_3) + \frac{\beta_{23}}{\sqrt{2}} (\sqrt{2}\, x_2 x_3). \end{aligned}$$

As before we denote by $\mathbf{X}$ the $N \times \frac{1}{2}(k + 1)(k + 2)$ matrix of independent variables corresponding to $\mathbf{D}$. If the set of points is submitted to some rotation the new design matrix will be $\mathbf{DH}$ where $\mathbf{H}$ is $k \times k$ orthogonal matrix. The matrix of independent variables will be transformed to $\dot{\mathbf{X}} = \mathbf{XG}$ where $\mathbf{G}$ is a matrix derived from $\mathbf{H}$ which when partitioned after the 1st and $(k + 1)$th row and column has the form

$$(67)\qquad \mathbf{G} = \left[\begin{array}{c|c|c} 1 & & \\ \hline & \mathbf{H} & \\ \hline & & \mathbf{H}^{[2]} \end{array}\right]$$

The partitioning will be seen to correspond to the separation of the constant term, first order coefficients and second order coefficients. The matrix $\mathbf{H}^{[2]}$ is the second Schläflian matrix derived from $\mathbf{H}$ which may itself be conveniently partitioned after its kth row and column and is of the form

$$(68)\qquad \mathbf{H}^{[2]} = \left[\begin{array}{c|c} \boldsymbol{\alpha} & \boldsymbol{\beta} \\ \hline \boldsymbol{\gamma} & \boldsymbol{\delta} \end{array}\right].$$

This partitioning corresponds to the separation of quadratic and interaction effects. For example, for $k = 3$

$$(69)\qquad \mathbf{H} = \begin{bmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & h_{33} \end{bmatrix};$$

then

(70) and (71)
$$\alpha = \begin{bmatrix} h_{11}^2 & h_{12}^2 & h_{13}^2 \\ h_{21}^2 & h_{22}^2 & h_{23}^2 \\ h_{31}^2 & h_{32}^2 & h_{33}^2 \end{bmatrix}, \qquad \beta = \begin{bmatrix} 2^{\frac{1}{2}}h_{11}h_{12} & 2^{\frac{1}{2}}h_{11}h_{13} & 2^{\frac{1}{2}}h_{12}h_{13} \\ 2^{\frac{1}{2}}h_{21}h_{22} & 2^{\frac{1}{2}}h_{21}h_{23} & 2^{\frac{1}{2}}h_{22}h_{23} \\ 2^{\frac{1}{2}}h_{31}h_{32} & 2^{\frac{1}{2}}h_{31}h_{33} & 2^{\frac{1}{2}}h_{32}h_{33} \end{bmatrix},$$

(72)
$$\gamma = \begin{bmatrix} 2^{\frac{1}{2}}h_{11}h_{21} & 2^{\frac{1}{2}}h_{12}h_{22} & 2^{\frac{1}{2}}h_{13}h_{23} \\ 2^{\frac{1}{2}}h_{11}h_{31} & 2^{\frac{1}{2}}h_{12}h_{32} & 2^{\frac{1}{2}}h_{13}h_{33} \\ 2^{\frac{1}{2}}h_{21}h_{31} & 2^{\frac{1}{2}}h_{22}h_{32} & 2^{\frac{1}{2}}h_{23}h_{33} \end{bmatrix},$$

(73)
$$\delta = \begin{bmatrix} h_{11}h_{22} + h_{12}h_{21} & h_{11}h_{23} + h_{13}h_{21} & h_{12}h_{23} + h_{13}h_{22} \\ h_{11}h_{32} + h_{12}h_{31} & h_{11}h_{33} + h_{13}h_{31} & h_{12}h_{33} + h_{13}h_{32} \\ h_{21}h_{32} + h_{22}h_{31} & h_{21}h_{33} + h_{23}h_{31} & h_{22}h_{33} + h_{23}h_{32} \end{bmatrix},$$

where the terms are arranged in the order shown in Eq. (66).

The original moment matrix is $N^{-1}\mathbf{X}'\mathbf{X}$. After rotation the moment matrix is $N^{-1}\dot{\mathbf{X}}'\dot{\mathbf{X}} = N^{-1}\mathbf{G}'\mathbf{X}'\mathbf{X}\mathbf{G}$. If the design is rotatable then the moment matrix before and after rotation are equal whatever the orthogonal matrix $\mathbf{H}$ from which $\mathbf{G}$ is derived. As we have seen, this implies that the matrix $N^{-1}\mathbf{X}'\mathbf{X}$ must be of a particular form. With the present definition of the interaction variables this form is

(74)
$$N^{-1}(\mathbf{X}'\mathbf{X}) = \begin{bmatrix} 1 & \cdot & \mathbf{1}' & \cdot \\ \cdot & \mathbf{I} & \cdot & \cdot \\ \mathbf{1} & \cdot & \lambda_4(2\mathbf{I} + \mathbf{1}\mathbf{1}') & \cdot \\ \cdot & \cdot & & 2\lambda_4\mathbf{I} \end{bmatrix},$$

where the dots indicate null submatrices, $\mathbf{I}$ is the identity matrix and $\mathbf{1}$ is a column vector with elements all unity. The partitioning in this and all moment matrices that follow is after the 1st, $(k+1)$th, and $(2k+1)$th row and column. This partitioning separates the elements corresponding to the constant term, the first order terms, the quadratic terms and the interaction terms respectively.

7.3 *Three dimensional designs.* In three dimensions sets of n points equally spaced on a sphere are provided by the vertices of the five regular figures. These are the tetrahedron ($n = 4$), the octahedron ($n = 6$), the cube ($n = 8$), the icosahedron ($n = 12$), and the dodecahedron ($n = 20$). Using the method of the previous section we can study the moment matrices for these sets of points subject to an arbitrary rotation.

For example, in the case of the tetrahedron we may suppose that initially the coordinates of its four vertices, i.e., the rows of $\mathbf{D}$, are $(-1, -1, 1)$, $(1, -1, -1)$, $(-1, 1, -1)$, and $(1, 1, 1)$. We can then write down the matrix of independent variables $\mathbf{X}$ for a second order model, the moment matrix $\frac{1}{4}\cdot\mathbf{X}'\mathbf{X}$ and finally the corresponding matrix $\frac{1}{4}\cdot\dot{\mathbf{X}}'\dot{\mathbf{X}} = \frac{1}{4}\cdot\mathbf{G}'\mathbf{X}'\mathbf{X}\mathbf{G}$ after an arbitrary rotation **H** has been applied to **D**. We thus obtain

$$\frac{1}{4}\cdot\dot{\mathbf{X}}'\dot{\mathbf{X}} = \left[\begin{array}{c|c|c|c} 1 & \cdot & \mathbf{1}' & \cdot \\ \hline \cdot & \mathbf{I} & \sqrt{2}\mathbf{H}'\mathbf{J}\boldsymbol{\gamma} & \sqrt{2}\mathbf{H}'\mathbf{J}\boldsymbol{\delta} \\ \hline \mathbf{1} & \sqrt{2}\boldsymbol{\gamma}'\mathbf{J}\mathbf{H} & \mathbf{1}\mathbf{1}' + 2\boldsymbol{\gamma}'\boldsymbol{\gamma} & 2\boldsymbol{\gamma}'\boldsymbol{\delta} \\ \hline \cdot & \sqrt{2}\boldsymbol{\delta}'\mathbf{J}\mathbf{H} & 2\boldsymbol{\delta}'\boldsymbol{\gamma} & 2\boldsymbol{\delta}'\boldsymbol{\delta} \end{array}\right],$$

Where **J** is a square matrix with unit elements along the diagonal running from the bottom left hand corner to the top right-hand corner and zero elements elsewhere.

In a similar way for the other regular figures with scales adjusted so that $\rho^2 = k = 3$ we consider equiradial points formed by the

6 vertices of the octahedron	$(\pm\sqrt{3}, 0, 0), (0, \pm\sqrt{3}, 0), (0, 0, \pm\sqrt{3})$,
8 vertices of a cube	$(\pm 1, \pm 1, \pm 1)$,
12 vertices of the icosahedron	$(0, \pm a, \pm b), (\pm b, 0, \pm a), (\pm a, 0, \pm b)$,
20 vertices of the dodecahedron	$(0, \pm c^{-1}, \pm c), (\pm c, 0, \pm c^{-1}), (\pm c^{-1}, \pm c, 0)$, $(\pm 1, \pm 1, \pm 1)$,

where $a = 1.473$, $b = 0.911$, and $c = 1.618$. For the octahedron and cube the moment matrices after applying the general rotation are obtained by setting $k = 3$ in the expressions:

(76)
$$\frac{1}{2k}\mathbf{X}'\mathbf{X} = \left[\begin{array}{c|c|c|c} 1 & \cdot & \mathbf{1}' & \cdot \\ \hline \cdot & \mathbf{I} & \cdot & \cdot \\ \hline \mathbf{1} & \cdot & k\boldsymbol{\alpha}'\boldsymbol{\alpha} & k\boldsymbol{\alpha}'\boldsymbol{\beta} \\ \hline \cdot & \cdot & k\boldsymbol{\beta}'\boldsymbol{\alpha} & k\boldsymbol{\beta}'\boldsymbol{\beta} \end{array}\right],$$

Octahedron

(77)
$$\frac{1}{2^k}\mathbf{X}'\mathbf{X} = \left[\begin{array}{c|c|c|c} 1 & \cdot & \mathbf{1}' & \cdot \\ \hline \cdot & \mathbf{I} & \cdot & \cdot \\ \hline \mathbf{1} & \cdot & \mathbf{1}\mathbf{1}' + 2\boldsymbol{\gamma}'\boldsymbol{\gamma} & 2\boldsymbol{\gamma}'\boldsymbol{\delta} \\ \hline \cdot & \cdot & 2\boldsymbol{\delta}'\boldsymbol{\gamma} & 2\boldsymbol{\delta}'\boldsymbol{\delta} \end{array}\right]$$

Cube

and for the icosahedron and dodecahedron by setting $n = 12$ and 20 respectively in the expression:

(78)
$$\frac{1}{n}\mathbf{X}'\mathbf{X} = \left[\begin{array}{c|c|c|c} 1 & \cdot & \mathbf{1}' & \cdot \\ \hline \cdot & \mathbf{I} & \cdot & \cdot \\ \hline \mathbf{1} & \cdot & \frac{3}{5}(2\mathbf{I} + \mathbf{1}\mathbf{1}') & \cdot \\ \hline \cdot & \cdot & \cdot & \frac{3}{5}(2\mathbf{I}) \end{array}\right].$$

As is to be expected, the vertices of the tetrahedron, octahedron, and cube do not individually supply rotatable sets of order 2 although they all provide rotatable sets of order 1. The larger number of points provided by the icosahedron and the dodecahedron however provide rotatable sets of order 2. These have of course the singular value of $\lambda_4 = \frac{3}{5}$.

As before therefore we may combine icosahedral and dodecahedral sets either with points in the center or with one another to form second order rotatable designs. These designs are built up in any one of the following ways:

(1) the 12 vertices of an icosahedron in any orientation with $n_1 \geqq 1$ points at the center,

(2) the 20 vertices of a dodecahedron in any orientation with $n_1 \geqq 1$ points at the center,

(3) the vertices of two concentric icosahedra of differing radii ρ_1 and ρ_2 each in any relative and absolute orientation,

(4) the vertices of two concentric dodecahedra of differing radii ρ_1 and ρ_2 each in any relative and absolute orientation,

(5) the vertices of an icosahedron of radius ρ_1 together with the vertices of a dodecahedron having the same center and radius ρ_2 each in any relative and absolute orientation.

The choice of n_1 in designs (1) and (2) and of ρ_1/ρ_2 in designs (3), (4), and (5) determines the value of λ_4 and hence via Eq. (48) the manner in which the variance of $\hat{y}$ changes with ρ. In particular, the value given in Table 1 for $k = 3$ is $\lambda_4 = 0.84$. This value is most nearly obtained (Eq. 59) with $n_1 = 5$ for design (1), $n_1 = 8$ for design (2). Also from Eq. (58), ρ_1/ρ_2 should be 2.11 for designs (3) and (4), and 2.85 or 0.530 for design (5).

As with the two dimensional designs, sets of points not themselves rotatable arrangements of order two may be combined to give second order rotatable designs. Of particular importance because of the existence of parallel designs in k dimensions are the designs obtained by combining the vertices of a concentric cube and octahedron. The relative orientation of the figures is such that each line joining the origin to a vertex of the cube pierces the center of a face of the octahedron and vice versa. These designs are special cases of the central composite designs described in references [1] and [13].

Since $\mathbf{H}^{[2]}$ is orthogonal

(79)
$$\boldsymbol{\alpha}'\boldsymbol{\beta} = -\boldsymbol{\gamma}'\boldsymbol{\delta}; \qquad \boldsymbol{\gamma}'\boldsymbol{\gamma} = \mathbf{I} - \boldsymbol{\alpha}'\boldsymbol{\alpha}; \qquad \boldsymbol{\beta}'\boldsymbol{\beta} = \mathbf{I} - \boldsymbol{\delta}'\boldsymbol{\delta}.$$

Using these identities, it will be seen from the nature of the moment matrices of the octahedron and cube (76) and (77) that by suitably choosing the relative sizes of the figures a combined arrangement can be obtained whose moment matrix is of the form (74) required for a rotatable design of second order. If ρ_a and ρ_c are the radii of circumscribing spheres of the octahedron and cube then $\rho_a/\rho_c = 2^{3/4}/3^{1/2} = 0.9710$ and $\lambda_4 = 0.6005$.

This value of λ_4 is very close to the singular value of $k/(k+2) = 0.6$. By adding points at the center however satisfactory values of λ_4 may be obtained. The value $\lambda_4 = 0.84$ given in Table 1 which gives the same precision at $\rho = 0$ as at $\rho = 1$ is most nearly obtained with 6 points at the center, and the value of $\lambda_4 = 1$ required for "orthogonality" is most nearly attained with 9 points at the center.

From the nature of the moment matrices in Eqs. (76), (77), and (78) it is seen that in general an infinity of three-dimensional second order rotatable designs can be generated by combining in various ways the vertices of octahedra, cubes, icosahedra and dodecahedra with or without added center points. One such design of considerable practical interest used by De Baun employs a cube with *two* added octahedra but no center points.

7.4 *Designs in more than* 3 *dimensions.* In five or more dimensions there exist only three regular figures. These are the regular simplex (k-dimensional analogue of the tetrahedron having $k + 1$ vertices), the cross-polytope (k-dimensional analogue of the octahedron having $2k$ vertices) and the measure polytope or hypercube (k-dimensional analogue of the cube having 2^k vertices). In four dimensions other regular figures occur. These have 24 vertices, 120 vertices, and 600 vertices. The figures with 120 and 600 vertices are of little interest from the point of view of constructing usable experimental designs and the figure with 24 vertices may be obtained by combining the cross polytope with the hypercube. Our discussion will therefore be confined to designs constructed from the vertices of the regular simplex, the cross polytope and the hypercube.

The regular simplex always supplies a first order rotatable design and we shall show that the cross polytope and hypercube can always be combined to give an arrangement from which a second order rotatable design may be obtained.

If we suppose the cross polytope and the hypercube each to have radius $k^{1/2}$ and to be in 'standard orientation' so that the $2k$ vertices of the cross polytope have coordinates

$$(\pm k^{1/2}, 0, 0, \cdots, 0)\ (0, \pm k^{1/2}, 0, \cdots, 0) \cdots, (0, 0, 0, \cdots, \pm k^{1/2})$$

and the 2^k vertices of the cube have coordinates $(\pm 1, \pm 1, \cdots, \pm 1)$ then the moment matrices, after applying the same rotation $\mathbf{H}$, are those given in Eqs. (76) and (77).

By combining the vertices of the cross polytope of radius ρ_a with those of the measure polytope of radius ρ_c in the relative orientation indicated so that $2k^2\rho_a^4 = 2^{k+1}\rho_c^4$, that is so that $\rho_a/\rho_c = 2^{k/4}/k^{1/2}$; an arrangement with the desired moment matrix (74) results.

These rotatable arrangements when combined together or augmented with suitable numbers of points at the center provide second order rotatable designs of great practical value. In their "standard orientation" the resulting designs are particular examples of the composite designs discussed in references [1] and [13] and consequently lend themselves very conveniently to sequential experimentation. As is discussed more fully in [1] they may be built up in parts each of which supplies valuable interim information. They are particularly simple to use. In standard orientation the part of the design corresponding to the measure polytope or hypercube defines a set of experimental points which follow the familiar 2^k factorial design. To form the second order rotatable designs these are augmented with points at the center and with points corresponding to the cross polytope in which all the variables except one are held in turn at the 'center' levels, the remaining variable being maintained first at a level above its center value and then at a level below its center value. Because in standard orientation the latter points lie along the coordinate axes they may be referred to as "axial points".

When k is sufficiently large a suitable fractional replicate can replace the full hypercube. Since a second order moment matrix identical with that of the full factorial will be obtained with any fractional replicate of the 2^k design in which no effects of second order or lower order are confounded. The only result of this substitution will be to effect the alias matrix of the design.

For a k dimensional design with $n_a = 2k$ axial points, $n_c = 2^{(k-p)}$ points in the $(\frac{1}{2})^p$ replicate of the 2^k factorial, and n_0 points at the center, $\rho_a/\rho_c = n_c^{1/4}/k^{1/2}$ and

$$\lambda_4 = N/\{n_c + 4(1 + n_c^{1/2})\}, \tag{81}$$

where $N = n_a + n_c + n_0$.

When using these designs in their standard orientation it is simplest to regard them as scaled so that the hypercube or fractional hypercube has its coordinates equal to plus or minus unity. The N coordinates of the complete design are then

n_c points (2^k factorial or suitable fraction): $(\pm 1, \pm 1, \cdots, \pm 1)$,
n_a points (axial points): $(\pm\alpha, 0, 0, \cdots, 0)$, $(0, \pm\alpha, 0, \cdots, 0)$, $\cdots$, $(0, 0, \cdots, \pm\alpha)$,
n_0 points (center conditions): $(0, 0, 0, \cdots, 0)$.

Then $\alpha = n_c^{1/4}$ and the scale factor c of Eq. (3) is $N/(n_c + 2n_c^{1/2})$. The values of n_c, n_a, n_0, α, ρ_a/ρ_c and λ_4 for second order rotatable designs, which give the values of λ_4 set out in Table 1 and for orthogonal designs, are given in the Table 3 for $k = 2, 3, 4, \cdots, 8$ dimensions.

8. Arrangement of the designs in blocks. To avoid bias due to systematic disturbances the complete set of experimental trials corresponding to the points which form the design could be performed in random order. Frequently however it is possible to carry out limited groups of trials under more homogeneous conditions than can be attained for the complete set. It may then be possible to achieve greater accuracy by performing the designs in blocks, carrying out the individual trials within each block in random order. A block may for example refer to a group of experiments performed on the same day, or a group of experiments for which it was possible to use the same batch of starting material.

TABLE 3

Central composite rotatable second order designs

k	2		3		4		5		5($\frac{1}{2}$ rep)		6		6($\frac{1}{2}$ rep)		7		7($\frac{1}{2}$ rep)		8		8($\frac{1}{2}$ rep)		8($\frac{1}{4}$ rep)	
n_c	4		8		16		32		16		64		32		128		64		256		128		64	
n_a	4		6		8		10		10		12		12		14		14		16		16		16	
n_0 (Table 1)	5		6		7		10		6		15		9		21		14		28		20		13	
n_0 (Orthogonal)		8		9		12		17		10		24		15		35		22		52		33		20
N total	13	16	20	23	31	36	52	59	32	36	91	100	53	59	163	177	92	100	300	324	164	177	93	100
$\alpha = n_c^{\frac{1}{4}}$:	1.414		1.682		2.000		2.378		2.000		2.828		2.378		3.364		2.828		4.000		3.364		2.828	
λ_4 Table 1	0.81		0.86		0.86		0.89		0.89		0.91		0.90		0.92		0.92		0.93		0.93		0.93	
λ_4 Orthogonal		1		0.99		1		1.01		1		1		1.01		1.00		1		1		1.00		1
ρ_a/ρ_c	1.000		0.971		1.000		1.064		0.894		1.155		0.971		1.271		1.069		1.414		1.189		1.000	

We shall show how the designs we have discussed may be performed in orthogonal blocking arrangements. On the usual assumption, that the effect of carrying out a particular trial in one block rather than another is merely to change the expected value of the response by a fixed amount which depends only on the particular blocks involved, such arrangements insure that the estimated coefficients of the polynomial are completely independent of the block differences and their standard errors depend on the within-block variance only.

For N experimental points assigned to m blocks with n'_w points in the wth block we suppose that

$$\eta_u = \sum_{w=1}^{m} \beta_{0w} z_{wu} + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i=1}^{k} \sum_{j=i}^{k} \beta_{ij} x_{iu} x_{ju} ,$$

where β_{0w} is the expected value of the response in the wth block at the experimental conditions corresponding to the origin of the design, and z_{wu} is a "dummy" variable taking the value unity for those experimental points which fall in the wth block and zero for all other experimental points. We shall call x_i, $x_i x_j$, etc., the polynomial variables and z_v, z_w, etc., the block variables.

In whatever manner the experimental points are assigned to the blocks we can except in the "pathological" cases detailed below estimate the coefficients of the polynomial equation allowing for the block effects, by the method of least squares. However the manner in which the experimental points are assigned to the blocks profoundly affects the efficiency of estimation and the ease with which the estimates are calculated. In particular, if it is possible so to allocate the experimental points to the blocks that the block variables and polynomial variables are orthogonal, then the inclusion of blocks does not at all influence the estimation of the polynomial coefficients and the only effect of blocking is the wholly desirable one of limiting the experimental error to that occurring within blocks. The analysis of the experiment proceeds exactly as if there were no blocking, except that in the estimation of the residual error the contribution due to blocks is subtracted from the residual sum of squares.

In order to find the conditions that must be satisfied to allow orthogonal blocking it is simplest to rewrite the model in the equivalent form

$$\eta_u = \beta_0 + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i=1}^{k} \sum_{j=i}^{k} \beta_{ij} x_{iu} x_{ju} + \sum_{w=1}^{m} \delta_w (z_{wu} - \bar{z}_w), \tag{82}$$

$$\beta_0 = \sum_{w=1}^{m} \frac{n'_w}{N} \beta_{0w} , \qquad \delta_w = \beta_{0w} - \beta_0 , \qquad \bar{z}_w = n'_w / N,$$

We note that $z_{wu} - \bar{z}_w$ is equal to $1 - n'_w/N$ when the uth set of conditions is in the wth block, and to $-n'_w/N$ otherwise.

The conditions for orthogonal blocks, that is to say the conditions that the block variables $z_{wu} - \bar{z}_w$ shall be orthogonal to the variables

$$x_0 , x_1 , x_2 , \cdots x_k , x_1^2 , x_2^2 , \cdots x_k^2 , x_1 x_2 , \cdots , x_{k-1} x_k$$

in the second degree polynomial, can be written

$$\sum_{u=1}^{N} x_{iu} x_{ju}(z_{wu} - \bar{z}_w) = 0, \qquad (i, j = 0, 1, \cdots, k) \tag{83}$$

that is

$$\sum_{u=1}^{N} x_{iu} x_{ju} z_{wu} = \bar{z}_w \sum_{u=1}^{N} x_{iu} x_{ju}. \tag{84}$$

Now for any second order rotatable design, if $i \neq j$, $\sum_{u=1}^{N} x_{iu}x_{ju} = 0$, whence for orthogonal blocking we require

$$\sum_{u}^{n_w'} x_{iu} x_{ju} = 0, \qquad i \neq j, w = 1, 2, \cdots m, \tag{85}$$

where the summation includes only those values of u in the wth block. *Thus (1) all the sums of products between x_0, x_1, $\cdots$, x_k must be zero for each block.*

A second condition arises from putting $i = j$ in (84) whence

$$\frac{\sum_{u}^{n_w'} x_{iu}^2}{\sum_{u=1}^{N} x_{iu}^2} = \frac{n_w'}{N}, \tag{86}$$

where the summation in the numerator again is for those values of u in the wth block. *Hence* (2) *the fraction of the total sum of squares for each variable contributed by each block must be proportional to the number of observations in each block.*

8.1 *Examples of orthogonal blocking with designs based on equiradial sets of points.* Where the rotatable design consists of an equiradial set of points with added points at the center, we can satisfy both conditions (85) and (86) if we can divide the equiradial set into subsets which are themselves first order rotatable (i.e., first order orthogonal) designs. When this is possible the sum of squares for each variable in each subset will be proportional to the number of points in the subset, and we have only to add a number of center points to each subset proportional to the number of points it already possesses to obtain a orthogonal block.

For example, consider a two dimensional "hexagonal" design consisting of 6 points at the vertices of a hexagon together with $2p$ center points. We can perform this design in two orthogonal blocks each consisting of three points at the vertices of an equilateral triangle and the remaining p points at the center. Similarly an octagonal design (the two dimensional rotatable composite design of Table 3) can be divided into two sets of four points at the vertices of a square with equal number of center points added to each to form two blocks. A "nonagonal" design may be divided into three equilateral triangles, which form the basis of three blocks and so on.

In three dimensions the vertices of the dodecahedron may be divided into five sub-sets each of which comprise the vertices of a tetrahedron. Thus for example a design consisting of twenty points at the vertices of the dodecahedron plus $5p$ points at the center is divisable into five orthogonal blocks of $4 + p$ points. Each block consists of a complete tetrahedron plus p center points.

8.2 *Blocking with composite rotatable designs.* The important composite rotatable designs lend themselves very conveniently to blocking and some valuable work on this topic has been carried out independently by De Baun [15]. Because the number of center points in any block must be an integer, exact rotatability and exact orthogonality between quadratic variables and block variables is not always attainable. We can however insure that either one of these desiderata is exactly satisfied and the other one nearly so. Although the extra labor involved in the calculations due to the slight non-orthogonality is not very great and the loss of efficiency is negligible, it is simplest in practice to use designs in which the block effects are exactly orthogonal but the condition of rotatability is slightly relaxed.

The central composite design in standard orientation consists of n_c points at the vertices of a cube corresponding to a 2^k factorial arrangement or some suitable fraction of it with coordinates $(\pm 1, \pm 1, \cdots, \pm 1)$, together with $n_a = 2^k$ "axial" points with coordinates $(\pm\alpha, 0, \cdots, 0)$, $(0, \pm\alpha, \cdots, 0)$, $\cdots$, $(0, 0, \cdots, \pm\alpha)$, and n_0 points at the center with coordinates $(0, 0, \cdots, 0)$. If $\alpha = n_c^{1/4}$ the design is rotatable, but let us for the moment not assume that this is so.

The sets of points at the vertices of the cube and the set of the axial points are each first order rotatable designs. These two parts of the design thus provide a basis for a first division of the composite design into two blocks. The blocking will be orthogonal if it is possible to allocate the center points to the two parts so that the total number of points in each part is proportional to the sum of squares for each variable contributed by that part. If n_{c0} and n_{a0} are the numbers of center points in the cubic part and the axial part respectively then we require

$$\frac{2\alpha^2}{n_c} = \frac{n_a + n_{a0}}{n_c + n_{c0}}; \tag{87}$$

thus for any composite design with

$$\alpha = \left\{\frac{n_c(n_a + n_{a0})}{2(n_c + n_{c0})}\right\}^{1/2} \tag{88}$$

we obtain orthogonal blocking. Now for rotatability $\alpha = n_c^{1/4}$ and hence to achieve both orthogonal blocking and rotatability we require that

$$\frac{n_c^{1/2}}{2} = \frac{n_c + n_{c0}}{n_a + n_{a0}}. \tag{89}$$

The set of axial points cannot be further sub-divided into sets which are first order rotatable designs. Such sub-division is possible however for the set of points at the vertices of the cube provided a system of confounding for the two-level factorial or fractional factorial design exists such that all the comparisons confounded correspond to interactions between three or more variables. If this is so the comparisons confounded will be unassociated with the comparisons used to estimate the coefficients of the polynomial. Also, since the comparisons confounded are the defining contrasts of the sub-sets regarded as fractional factorials and correspond to interactions between three or more factors, it follows that the sub-sets are individually first order rotatable designs. If the cube is divided up into sub-sets each containing the same number of points then in accordance with Eq. (86) we must add an equal number of center points to each sub-set to maintain orthogonality.

8.3 *Examples.*

(i) We first consider the four-dimensional design to illustrate the situation where both rotatability and orthogonality of blocking may be attained. From Table 4 it is seen that in standard orientation this design consists of the 2^4 factorial, with coordinates $(\pm 1, \pm 1, \pm 1, \pm 1)$, 8 axial points at distance $\alpha = 16^{1/4} = 2$ units from the center, and to approximately satisfy the requirement of Table 1 seven points added at the center.

We can achieve orthogonal blocking and rotatability if we can satisfy Eq. (89) which gives

$$2 = \frac{16 + n_{c0}}{8 + n_{a0}}. \tag{90}$$

Now the total number of points at the center $n_0 = n_{c0} + n_{a0}$ is not critical and if, for example we use six points at the center instead of seven the only effect will be to slightly change the variance function and in particular to decrease slightly the precision near the origin. If we now allocate $n_{c0} = 4$ points to the cube and $n_{a0} = 2$ points to the axial part, we satisfy (90). In this way the complete set of $16 + 8 + 6 = 30$ points is divided into two orthogonal blocks, one containing $16 + 4 = 20$ points and one with $8 + 2 = 10$ points. Now the 2^4 factorial designs corresponding to the cube may be further divided into two halves each of which is a rotatable design of order 1. This may be done without affecting the estimation of the polynomial coefficients by arranging that the contrast between the two halves corresponds to a three or four-factor interaction. The most suitable contrast is the four-factor interaction and to effect the division we allocate those points in the design for which the product $x_1x_2x_3x_4$ is 1 to one part and those for which it is -1 to the other. We may in accordance with Eq. (86) maintain orthogonal blocking by dividing the four center points assigned to the cube equally between the parts, two to each half. Finally therefore the design of 30 points is carried out in 3 blocks each of ten points consisting of the axial points together with two center points and the two half-replicates of the cube each with two center points. The blocking is completely orthogonal and the design exactly rotatable. It should be noted that since the separate blocks are themselves first order rotatable designs, this scheme ensures orthogonal blocking not only in the standard orientation of the design which we have specifically discussed but also in every other orientation.

(ii) To illustrate the situation where orthogonality of blocking and rotatability are not exactly attainable simultaneously, consider the three-dimensional composite design. From Table 3 we see that, in standard orientation, the design consists of the 2^3 factorial with coordinates $(\pm 1, \pm 1, \pm 1)$, the six axial points each at a distance $8^{1/4} = 1.6818$ and about six center points are needed to satisfy approximately the requirements of Table 1. From (89), to achieve orthogonal blocking and rotatability we require

$$\frac{8^{1/2}}{2} = \frac{8 + n_{c0}}{6 + n_{a0}}, \tag{91}$$

where $n_{c0} + n_{a0}$ is about 6. We come nearest to satisfying this requirement by putting $n_{c0} = 4$ and $n_{a0} = 2$; however, since the equation cannot be exactly satisfied with integral values, some slight nonorthogonality must occur. This non-orthogonality would be the same in every orientation of the design and the estimates of the coefficients corrected for block effects would in fact be very easily obtained without much extra labor. However since *exact* rotatability is not required in practice we choose therefore to adjust the value of α to obtain orthogonality at the expense of rotatability. From Eq. (88) it is seen that for $n_{c0} = 4$, $n_{a0} = 2$ and for orthogonal blocking we require

$$\alpha = \left\{\frac{8(8)}{2(12)}\right\}^{1/2} = 1.6330 \tag{92}$$

instead of $\alpha = 1.6818$ required for rotatability. For this value of α the variance contours will not be exact spheres, the difference from sphericity will however be so slight as to be of no practical importance. Since the sub-groups are first order rotatable designs the blocking will remain orthogonal in every orientation. The elements corresponding to the constant terms and second order terms in both the moment matrix and the precision matrix will change slightly as the design is rotated however.

As before the cube part may be divided into two portions. These are the two fractional replicates whose defining contrast is the three-factor interaction. Since four center points are allocated to the cube we can divide these equally between the fractions and so maintain orthogonality.

Finally therefore the 20 points of the design with $\alpha = 1.6330$ may be divided into three orthogonal blocks. One block consists of eight points containing the six axial points and two of the center points, and other two blocks each contain a half replicate of the cube together with two center points. A list of orthogonal blocking arrangements for rotatable and near-rotatable composite designs is given in Table 4 below.

An aspect which makes these blocking arrangements particularly useful arises out of the nature of the situation in which these designs are often used. In the exploration of response surfaces [1], [13] trials are usually performed sequentially and often have as their object the increase or maximization of some response. It has been shown that each block of the second order design is itself a first order rotatable design with added points at the center. Such a design allows estimates to be obtained not only of first order effects but also (assuming a second order equation is adequate to represent the surface) of the *sum* of the quadratic effects. For if $\bar{y}_0$ is the mean of the observations of the center and $\bar{y}_d$ the mean of the observations in the first order design then using (8a) it will be found that for any

TABLE 4

Blocking arrangements for rotatable and near-rotatable central composite design

k	2*	3	4	5	5(½ rep)	6	6(½ rep)	7	7(½ rep)
Blocks within cube									
n_c : Number of points in cube	4	8	16	32	16	64	32	128	64
Number of blocks in cube	1	2	2	4	1	8	2	16	8
Number of points in block from cube	4	4	8	8	16	8	16	8	8
Number of added center points	3	2	2	2	6	1	4	1	1
Total number of points in block	7	6	10	10	22	9	20	9	9
Axial block									
n_a Number of axial points	4	6	8	10	10	12	12	14	14
Number of added points	3	2	2	4	1	6	2	11	4
Total number of points in block	7	8	10	14	11	18	14	25	18
Grand total of points in the design	14	20	30	54	33	90	54	169	80
Value of α for orthogonal blocking	1.4142	1.6330	2.0000	2.3664	2.0000	2.8284	2.3664	3.3636	2.8284
Value of α for rotatability	1.4142	1.6818	2.0000	2.3784	2.0000	2.8284	2.3784	3.3333	2.8284

* A more economical design for $k = 2$ (which is not however a composite design as here defined) is that mentioned in Section 7.1, in which 6 points at the vertices of a hexagon are divided into two sets of three points. To attain the value of λ_4 given in Table 1 two points are added to each set to form two blocks.

first order rotatable design in any orientation (that is, for any orthogonal first order design),

$$\mathcal{E}(\bar{y}_d - \bar{y}_0) = \sum_{i=1}^{k} \beta_{ii} .$$

In the neighborhood of a true maximum $\bar{y}_d - \bar{y}_0$ is not small relative to the linear coefficients b_i and this provides an additional indication of the inadequacy of a linear model.

For example suppose that four variables were studied with the intention of finding an optimum set of conditions using the methods of Box and Wilson [1]. A half replicate of the 2^4 design with two center points could first be run in random order. This design would supply estimates of the four first order terms β_1, β_2, β_3, and β_4 and combinations of the interaction terms namely $(\beta_{12} + \beta_{34})$, $(\beta_{13} + \beta_{24})$, $(\beta_{14} + \beta_{23})$ and of the sum of the four quadratic terms $\sum \beta_{ii}$. If first order terms were dominant, progress could probably be made without a more elaborate design and moves in the indicated direction of increasing yield would be made until improvement in that direction was exhausted. At this point a new first order design would be begun at the improved set of conditions.

If the first order terms were not dominant, or if more precision were needed, or a tentative move had not met with success, the second half of the factorial design together with two further center points could be carried out, and the situation again reviewed in the light of the set of 20 trials now available. Finally, if the evidence indicated that further progress could be attained only by fitting the second degree equation, the third block of ten experiments consisting of the axial points and two center points would be added. The complete set of 30 trials could then be used to provide efficient estimates of the best fitting second degree equation and further progress would follow.

9. Details of calculations using the designs. From the observations generated by the second-order designs least squares estimates of the coefficients of the fitted polynomial, together with their variances and the appropriate analysis of variance table, are readily computed.

9.1 *Estimates of the coefficients and of their standard errors.* To estimate the coefficients we require only the sums of products of the observations with the independent variables. We shall use the notation

$$\sum_{u=1}^{N} x_{0u} y_u = \{0\ y\}, \qquad \sum_{u=1}^{N} x_{iu} y_u = \{i\ y\}, \qquad \sum_{u=1}^{N} x_{iu} x_{ju} y_u = \{i\ j\ y\},$$

where $i, j = 1, 2, \cdots, k$.

(i) *Rotatable designs.* The form of the inverse matrix for any rotatable design is given by (44) whence we have for any k-dimensional second order rotatable design with parameter λ_4

$$(93)\quad b_0 = AN^{-1}[2\lambda_4^2(k+2)\{0\ y\} - 2\lambda_4 c \textstyle\sum_{i=1}^{k} \{i\ i\ y\}],$$

$$(94)\quad b_i = cN^{-1}\{i\ y\},$$

$$(95)\quad b_{ii} = AcN^{-1}[c[(k+2)\lambda_4 - k]\cdot\{i\ i\ y\} + c(1-\lambda_4)\textstyle\sum_{j=1}^{k} \{j\ j\ y\} - 2\lambda_4\{0\ y\}],$$

$$(96)\quad b_{ij} = c^2N^{-1}\lambda_4^{-1}\{i\ j\ y\},$$

where

$$(97)\qquad A = [2\lambda_4\{(k+2)\lambda_4 - k\}]^{-1}$$

and the scale factor

$$(98)\qquad c = N/\textstyle\sum_{u=1}^{N} x_{iu}^2 .$$

Again using (44) the variances of the estimates are

$$(99)\qquad V(b_0) = 2A\lambda_4^2(k+2)\sigma^2/N,$$

(100) $$V(b_i) = c\sigma^2/N,$$

(101) $$V(b_{ii}) = A\{(k+1)\lambda_4 - (k-1)\}c^2\sigma^2/N,$$

(102) $$V(b_{ij}) = c^2\sigma^2/N\lambda_4 .$$

These formulae apply to any rotatable design. For the particular case of the rotatable central composite designs scaled so that in standard orientation the coordinates of the n_c points forming the two-level factorial or fractorial factorial part are $(\pm 1, \pm 1, \cdots, \pm 1)$ the value of the scale factor c is $N/(n_c + 2n_c^{1/2})$.

(ii) *Central composite designs not necessarily rotatable.* In order to obtain exactly orthogonal blocking for the central composite designs, we have proposed certain arrangements which are not exactly rotatable. For any central composite design the estimates of the coefficients and their variances are readily computed and these are of course unaffected by orthogonal blocking.

The non-diagonal elements of the moment matrix for any central composite design in standard orientation are zero apart from terms arising from cross products between the "constant term" variable x_0 and the quadratic variables $x_i^2 (i = 1, 2, \cdots, k)$. The sub-matrix of the moment matrix corresponding to these variables is of the form

(103) $$\begin{bmatrix} d & e & e & e & \cdots & e \\ e & f & g & g & \cdots & g \\ e & g & f & g & \cdots & g \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ e & g & g & g & \cdots & f \end{bmatrix}$$

The reciprocal of this matrix is of the same form. Denoting its elements in corresponding positions by capital letters we find

(104) $$D = H^{-1}\{f + (k-1)g\}(f-g),$$

(105) $$E = -H^{-1}e(f-g),$$

(106) $$F = H^{-1}\{df + (k-2)\,dg - (k-1)e^2\},$$

(107) $$G = H^{-1}(e^2 - dg),$$

(108) $$H = (f-g)\{df + (k-1)\,dg - ke^2\}.$$

For the composite designs in conventional scaling

(109) $$d = N, \qquad e = n_c + 2\alpha^2, \qquad f = n_c + 2\alpha^4, \qquad g = n_c .$$

Using (109) with (104), (105), (106), (107), and (108) the estimated coefficients are readily calculated from the formulae

(110) $$b_0 = D\{0\,y\} + E\textstyle\sum_{i=1}^{k} \{i\,i\,y\},$$

(111) $$b_i = (n_c + 2\alpha^2)^{-1}\{i\,y\},$$

(112) $$b_{ii} = E\{0\,y\} + F\{i\,i\,y\} + G\sum_{i\neq j}^{k} \{j\,j\,y\},$$

(113) $$b_{ij} = n_c^{-1}\{i\,j\,y\}.$$

The standard errors of these estimates are

(114) $$V(b_0) = D\sigma^2,$$

(115) $$V(b_i) = (n_c + 2\alpha^2)^{-1}\sigma^2,$$

(116) $$V(b_{ii}) = F\sigma^2,$$

(117) $$V(b_{ij}) = n_c^{-1}\sigma^2.$$

In practice we normally estimate σ from the data in the manner described below.

9.2 *Analysis of variance.* The total sum of squares $\sum_{u=1}^{N} y_u^2 = S$ having N degrees of freedom may be split into two parts: (i) The sum of squares S_{012} attributable to the fitted second degree equation having $(\frac{1}{2})(k + 2)(k + 1)$ degrees of freedom. This is given by

(118) $$S_{012} = b_0\{0\,y\} + \sum_{i=1}^{k} b_i\{i\,y\} + \sum_{i=1}^{k}\sum_{j=i}^{k} b_{ij}\{i\,j\,y\}.$$

(ii) the "overall" residual sum of squares R having $N - (\frac{1}{2})(k + 2)(k + 1)$ degrees of freedom which is obtained by difference

(119) $$R = S - S_{012}.$$

Each of these sums of squares may be further subdivided.

9.21 *Analysis of sum of squares due to regression.* The sum S_{012} may be divided into three parts:

(i) The sum S_0, having one degree of freedom attributable to the fitting of a polynomial of zero-th degree (the so-called "correction due to the mean")

(120) $$S_0 = \{0\,y\}^2/N.$$

(ii) The sum $S_{1.0}$ having k degrees of freedom. This is the "extra" sum of squares associated with the fitting of a first degree polynomial. Since, for the designs we have considered, b_0 is uncorrelated with any of the b_i

(121) $$S_{1.0} = \sum_{i=1}^{k} b_i\{i\,y\}.$$

(iii) The sum $S_{2.10}$ having $\frac{1}{2}k(k + 1)$ degrees of freedom, the "extra" sum of squares associated with the fitting of a second degree polynomial. Since for the designs we consider the b_i's are uncorrelated with b_0 and with the b_{ii}'s

(122) $$S_{2.10} = b_0\{0\,y\} + \sum_{i=1}^{k}\sum_{j=i}^{k} b_{ij}\{i\,j\,y\} - \{0\,y\}^2/N.$$

In specific examples other sub-divisions may be relevant. For instance, it might be suspected that a particular variable x_i had no effect at all on the result. In this case it would be appropriate to isolate a sum of squares S_i associated with the variable x_i. This could be done most conveniently by carrying out an analysis omitting x_i and $x_i x_j$ $(j = 1, 2, \cdots, k)$ from the model. The sum of squares associated with the reduced model would then be subtracted from the sum of squares associated with the full model to give S_i.

9.22 *Analysis of residual sum of squares.* Where blocking has not been used the overall residual sum of squares R may be analysed into two parts:

(i) The sum

$$S_E = \sum_{u=1}^{n_0} (y_{u0} - \bar{y}_0)^2, \tag{123}$$

where y_{u0} is the uth repeated observation at the center of the design and $\bar{y}_0$ is the mean of the observations at the center. This sum of squares has $n_0 - 1$ degrees of freedom and $S_E/(n_0 - 1)$ provides an estimate of the experimental error variance σ^2 on the assumption that this variance is independent of the levels of the variables x_i.

(ii) $R - S_E$ having $N - (\frac{1}{2})(k + 2)(k + 1) - n_0 + 1$ degrees of freedom, the residual sum of squares which measures experimental error together with lack of fit of the assumed form of equation. When the corresponding mean square is large compared with the estimate of pure error obtained in (i) above, this implies that the assumed form of the equation is inadequate. A full discussion will be found in [16] and will be published elsewhere.

9.23 *Analysis when blocking is employed.* When blocking is employed a further sum of squares S_B due to blocks is extracted so that the residual sum of squares R is now divided into three parts:

(i) S_B having $B - 1$ degrees of freedom

$$S_B = \sum_{b=1}^{B} n_b(\bar{y}_b - \bar{y})^2, \tag{124}$$

where B is the number of blocks, n_b is the number of observations in the bth block and $\bar{y}_b$ is the mean of the observations in the bth block.

(ii) The sum of squares S_E corresponding to pure error and having $n_0 - B$ degrees of freedom. This is the sum of the individual sums of squares for repeated observations at the center of each block

(iii) $R - S_B - S_E$ the residual which measures experimental error plus lack of fit.

The designs discussed are extremely convenient to use. The points at the center of the design allow a check to be made at a standard set of conditions while the experiment is being carried out and so helps to show up gross errors. Furthermore the center points provide an estimate of pure error from which it is possible to check the adequacy of the assumed form of equation without replicating the whole design.

10. Simplification of confidence region for maximum. On the assumption that a second degree equation can adequately represent a response surface in the region of interest, a confidence region for the stationary point of this surface has been derived in [17]. Unfortunately the boundary of the confidence region is, in general, not easy to compute but Wallace [20] has devised valuable approximations which are easy to compute and to appreciate. A very considerable simplification in the expression for the exact confidence interval occurs when a rotatable design is used to generate the experimental data.

Suppose the second degree equation in k variables $x_1, \cdots, x_i, \cdots, x_j, \cdots, x_k$ which has been fitted by least squares is written in the form

$$y - a_{00} = \mathbf{x}'\mathbf{a}_0 + (\tfrac{1}{2})\mathbf{x}'\mathbf{A}\mathbf{x}, \tag{125}$$

where $\mathbf{a}_0$ is the $k \times 1$ vector $\{a_{i0}\}$ and $\mathbf{A}$ is the $k \times k$ matrix $\{a_{ij}\}$ and in terms of the notation previously adopted $a_{00} = b_0$, $a_{i0} = b_i$, $\frac{1}{2}a_{ii} = b_{ii}$, $a_{ij} = b_{ij}$.

The position of the center of the fitted system is obtained by equating to zero the elements of the $k \times 1$ vector $\boldsymbol{\delta}$ defined by

$$\boldsymbol{\delta} = \mathbf{a}_0 + \mathbf{A}\mathbf{x}. \tag{126}$$

Thus if $\mathbf{x}_0$ is the vector of the k coordinates of this center then

$$\mathbf{a}_0 = -\mathbf{A}\mathbf{x}_0, \tag{127}$$

at which point the value of y is given by the equation

$$y_0 = a_{00} + (\tfrac{1}{2})\mathbf{x}_0'\mathbf{a}_0. \tag{128}$$

The confidence region given in [17] is defined by the inequality:

$$\boldsymbol{\delta}'\mathbf{V}^{-1}\boldsymbol{\delta} \leqq s^2 k F_\alpha(k, \varphi), \tag{129}$$

where $\mathbf{V}\sigma^2 = \mathcal{E}(\boldsymbol{\delta}'\boldsymbol{\delta})$, s^2 is an estimate of variance having φ degrees of freedom and distributed as $\chi^2\sigma^2/\varphi$ independently of $\boldsymbol{\delta}$, and $F_\alpha(k, \varphi)$ is the α probability point of the F distribution having k and φ degrees of freedom.

For a rotatable design using (100, 101, and 102), the variances and covariances of the δ's are given by

$$V(\delta_i) = N^{-1}\sigma^2(c + \lambda^{-1}c^2\rho^2 + \ell c^2 x_i^2), \qquad \text{Cov}(\delta_i\delta_j) = N^{-1}\sigma^2\ell c^2 x_i x_j, \tag{130}$$

where

$$\rho^2 = \sum_{i=1}^{k} x_i^2 \qquad \ell = \frac{k(\lambda - 1) + 2}{\lambda\{(k + 2)\lambda - k\}}, \tag{131}$$

c is the scale factor for the design defined in (3), and $\lambda = \lambda_4$. Thus

$$N\mathbf{V} = c(1 + \lambda^{-1}c\rho^2)\left\{\mathbf{I} + \frac{\ell c}{1 + \lambda^{-1}c\rho^2}\mathbf{x}\mathbf{x}'\right\}. \tag{132}$$

The matrix $\mathbf{V}$ is readily inverted using a theorem due to K. D. Tocher [18] to give

$$\mathbf{V}^{-1} = \frac{N}{c(1 + \lambda^{-1}c\rho^2)}\left\{\mathbf{I} - \frac{c\ell}{1 + (\lambda^{-1} + \ell)c\rho^2}\mathbf{x}\mathbf{x}'\right\}. \tag{133}$$

Thus

$$\boldsymbol{\delta}'\mathbf{V}^{-1}\boldsymbol{\delta} = \frac{N}{c(1+\lambda^{-1}c\rho^2)}\left\{\boldsymbol{\delta}'\boldsymbol{\delta} - \frac{c\ell}{1+(\lambda^{-1}+\ell)c\rho^2}(\boldsymbol{\delta}'\mathbf{x})^2\right\}. \tag{134}$$

Now using (126) with (127)

$$\boldsymbol{\delta} = \mathbf{A}(\mathbf{x} - \mathbf{x}_0). \tag{135}$$

It follows that when the data have been generated by a rotatable design the confidence region for the stationary point is given by the expression

$$\frac{N}{(1+\lambda^{-1}c\rho^2)}\left[\frac{1}{c}(\mathbf{x}-\mathbf{x}_0)'\mathbf{A}^2(\mathbf{x}-\mathbf{x}_0) - \frac{\ell}{1+(\lambda^{-1}+\ell)c\rho^2}\{(\mathbf{x}-\mathbf{x}_0)'\mathbf{A}\mathbf{x}\}^2\right] \leqq ks^2F_\alpha(k,\varphi). \tag{136}$$

Now a fitted second degree equation can be interpreted most readily by writing it in the canonical form

$$y - y_0 = \sum_{i=1}^{k} B_{ii}X_i^2. \tag{137}$$

The k elements B_{ii} are the latent roots of the matrix $(\frac{1}{2})\mathbf{A}$. If a diagonal matrix $\mathbf{B}$ is formed with the B_{ii} for its elements then the latent vectors of $\mathbf{A}$ form the k rows of an orthogonal matrix $\mathbf{M}$ such that

$$(\tfrac{1}{2})\mathbf{MA} = \mathbf{BM} \tag{138}$$

and the matrix $\mathbf{X}$ of "canonical variables" whose elements are $X_1, X_2, \cdots, X_k$ is defined by

$$\mathbf{X} = \mathbf{M}(\mathbf{x} - \mathbf{x}_0). \tag{139}$$

The coordinates of the initial origin $\mathbf{x} = \mathbf{0}$ in terms of the canonical variables is given by

$$\mathbf{X}_0 = -\mathbf{M}\mathbf{x}_0, \tag{140}$$

whence $\mathbf{x} = \mathbf{M}'(\mathbf{X} - \mathbf{X}_0)$. Thus the expression defining the confidence region reduces to the relatively simple expression

$$\frac{4N}{1+\lambda^{-1}c\rho^2}\left[\frac{1}{c}\sum_{i=1}^{k}B_{ii}^2X_i^2 - \frac{\ell}{1+(\lambda^{-1}+\ell)c\rho^2}\left\{\sum_{i=1}^{k}B_{ii}X_i(X_i - X_{i0})\right\}^2\right] \leqq ks^2F_\alpha(k,\varphi), \tag{141}$$

where

$$\rho^2 = \mathbf{x}'\mathbf{x} = (\mathbf{X}-\mathbf{X}_0)'\mathbf{MM}'(\mathbf{X}'-\mathbf{X}_0) = \sum_{i=1}^{k}(X_i - X_{i0})^2.$$

A rough delineation of the confidence region in a readily appreciated form can now be obtained by enumerating the points at which it cuts the canonical axes.

By direct substitution in (141) the point $(0, \cdots, 0, X_i, 0 \cdots 0)$ will be included in the confidence region provided that

$$B_{ii}^2 \leqq cks^2F_\alpha(k, \varphi)\left\{1 + \lambda^{-1}c \sum_{j \neq i}^{k} X_{j0}^2 + \lambda^{-1} c(X_i - X_{i0})^2\right\} \tag{142}$$
$$\times \frac{\left\{1 + (\lambda^{-1} + \ell)c \sum_{j \neq i}^{k} X_{j0}^2 + (\lambda^{-1} + \ell)c(X_i - X_{i0})^2\right\}}{4NX_i^2\left\{1 + (\lambda^{-1} + \ell)c \sum_{j \neq i}^{k} X_{j0}^2 + \lambda^{-1}c(X_i - X_{i0})^2\right\}}.$$

If the quantities $X_{10}, X_{20}, \cdots, X_{k0}$ are finite then as X_j tends to infinity this becomes

$$B_{ii}^2 \leqq (4N)^{-1}kF_\alpha(k, \varphi)\{\lambda^{-1} + \ell\}c^2s^2, \tag{143}$$

which is the condition that the confidence interval includes points at $\pm\infty$ on the canonical axis X_i

10.1 *Redundancy of canonical variables.* This result can be viewed from a somewhat different angle. In real problems one would expect (see for example reference [3]) that the underlying system would often be approximated by surfaces containing a stationary line, plane or hyperplane rather than a stationary point. When this occurred one or more of the B_{ii} calculated from the fitted equation would be close to zero and the corresponding canonical axes would delineate the stationary line, plane or space. Analysis of this sort is of considerable practical importance since it may help in the deduction of the underlying mechanism of the system [19].

An important question that normally arises is how small the canonical units B_{ii} must be before we may conclude that zero values are not inconsistent with the data. Now for any rotatable design the variances of the coefficients are the same in every orientation and since the B_{ii} are simply the "quadratic effects" in the directions of the canonical variables they have the same standard errors as have the quadratic effects b_{ii} before transformation. Were it not that the small values of the B_{ii} will be selected *because* they are small we might "test the significance" of the B_{ii} by dividing by their standard errors and referring the quotient to tables of the t distribution. Now the estimated variance of the quadratic coefficients selected from a rotatable design with scale factor c is $(4N)^{-1}$ $(\lambda^{-1} + \ell)c^2s^2$ and consequently the inequality (143) can be written

$$\left|\frac{B_{ii}}{\text{s.e. }(B_{ii})}\right| \leqq \sqrt{kF_\alpha(k, \varphi)}$$

implying that we can "test the significance" of the B_{ii} computed from a rotatable design by referring not to the t distribution but to the distribution of $kF_\alpha(k, \varphi)$.

This is a special case of a more general result derived by Wallace [20].

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