MULTI-FACTOR EXPERIMENTAL DESIGNS

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by

G. E. P. Box
J. S. Hunter

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Philadelphia Ordnance District
Department of the Army, Department of Defense
with
Institute of Statistics
North Carolina State College of
The University of North Carolina
Raleigh, North Carolina

Technical Supervisor
Ballistics Research Laboratories
Aberdeen Proving Ground
Aberdeen, Maryland

G. E. P. Box
J. S. Hunter
Authors of Report

1. INTRODUCTION

Suppose we have k quantitative factors whose levels are denoted by $X_1, X_2, \ldots, X_k$ on which depend the level of some response in accordance with an unknown relationship

$$\eta = \varphi(X_1, X_2, \ldots, X_k) \tag{1}$$

Suppose that in order to explore this relationship, N experiments are performed. The u^{th} of these experiments consists in adjusting the factor levels to a certain set of k pre-decided values, $X_{1u}, X_{2u}, \ldots, X_{ku}$ and of observing the response y_u. The problem of experimental design is that of deciding for given assumptions concerning the function φ what is the best arrangement of N sets of levels to use.

Following the convention adopted in previous papers we shall define a set of standardized factor levels

$$x_{iu} = \frac{(X_{iu} - \bar{X}_i)}{S_i} \qquad \text{where} \quad S_i = \left\{ \sum_{u=1}^{N} \frac{(X_{iu} - \bar{X}_i)^2}{N} \right\}^{1/2} \tag{2}$$

For these standardized levels therefore

$$\sum_{\substack{i=1\\ u=1}}^{N} x_{iu} = 0 \qquad \text{and} \qquad \sum_{\substack{i=1\\ u=1}}^{N} x_{iu}^2 = N \tag{3}$$

We shall denote by $\underline{D}$ the "design matrix" an N x k matrix which provides a program of N experiments to be performed. The elements of the u^{th} row of this matrix are the values of the standardized factor levels $x_{1u}, x_{2u}, \ldots, x_{ku}$ to be used in the u^{th} experiment. They also define the u^{th} experimental point in the k-dimensional factor space. Since the designs we consider will include many factors, they will be called multi-factor designs. By using standardized factor levels we may prepare a standard set of design matrices appropriate for various values of k, and for various types of assumptions concerning the function φ. In given circumstances, the experimenter could select the appropriate design matrix and (by deciding on suitable averages values $\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_k$ and units $S_1, S_2, \ldots, S_k$ which would cause the design to cover that region of the factor space in which he was interested) covert the standardized variables $x_1, x_2, \ldots, x_k$ of the design to the real levels $X_1, X_2, \ldots, X_k$ of the variables with which he is experimenting. The level of the i^{th} factor to be used in the u^{th} trial would then be $X_{iu} = \bar{X}_i + S_i x_{iu}$. We shall assume in what follows that we can approximate the function φ by means of its Taylor's Series in which terms up to degree d are included. That is to say, we will represent φ by a polynomial of degree d so that the response at the u^{th} point will be assumed to be given by

$$\eta_u = \beta_0 x_{0u} + \beta_1 x_{1u} + \ldots + \beta_k x_{ku} + \beta_{11} x_{1u}^2 + \ldots + \beta_{kk} x_{kk}^2 + \beta_{12} x_1 x_2 + \ldots + \beta_{k-1,k} x_{k-1} x_k \qquad (4)$$

with suitable choice of the coefficients β_0, β_1, etc. We shall obtain estimates b_0, b_1, etc. of these coefficients by fitting the equation to the N observed values of y at the N experimental points by the method of least squares.

We call β_i the i^{th} linear effect, and x_i the i^{th} linear independent variable, β_{ii} and x_i^2 the i^{th} quadratic effect and the i^{th} quadratic variable respectively, and β_{ij}, $x_i x_j$ the linear x linear interaction effect and variable for the i^{th} and j^{th} factors respectively, and so on. It is convenient to write the constant term as $\beta_0 x_{0u}$ rather than as β_0 defining x_{0u} as equal to unity for all values of u.

A design which includes k factors 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 $\binom{k+d}{k}$ terms so that a k-dimensional design of order d must contain at least this number of points, ie, $N \geq \binom{k+d}{k}$.

One arrangement of experiments that might be employed uses the points of intersection of a cubic lattice as the experimental points. Such arrangements are called factorial designs. A factorial design in which were determined all the effects of order d or less would require the performance of all combinations of d + 1 levels of the factors, thus $(d + 1)^k$ experiments would be required. The number of constants to be determined, and the number of observations required by the factorial designs are shown below

Order d of Design	k = 2	3	4	5	6	k = 2	3	4	5	6
1	3	4	5	6	7	4	8	16	32	64
2	6	10	15	21	28	9	27	81	243	729
3	10	20	35	56	84	16	64	256	1024	4096
4	15	35	70	116	200	25	125	625	3125	13625
	Number of Constants					Number of obs in factorial design				

The number of observations needed by the factorial design may sometimes be considerably reduced by fractional replication (particularly for first order designs when two-level fractional factorials may be employed). However this device is less effective for designs of higher order. There is also some doubt as to whether the relative emphasis placed on different terms in the series, as measured by the variances of the effects, is an ideal one with such designs. Since for quantitative factors there seems no prior reason for basing experimental arrangements on the factorial pattern some more fundamental approach may be attempted.

2. ORTHOGONAL DESIGNS

The problem of determining most efficient designs of order one has been discussed elsewhere (Box, 1952). The most important practical problem outstanding is that of investigating designs of order two which are of great importance in the study of near-stationary regions of the factor space, that is, regions in which the first order effects are small. We shall not, however, for the moment, limit the discussion to this special case.

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

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

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

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

The variances and co-variance of these effects are

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

where $\underline{C}^{-1}$ may be called the "precision" matrix.

An unbiased estimate of σ^2 is provided by the quantity

$$(N - L)^{-1}(\dot{\underline{Y}} - \underline{Y})'(\dot{\underline{Y}} - \underline{Y}) = (\underline{Y}'\underline{Y} - \underline{B}'\underline{X}'\underline{XB})(N-L)^{-1} \tag{8}$$

The expressions in (6), (7), and (8) contain the matrix $\underline{C} = [X'X]$ of sums of squares and products of the independent variables. We also notice that $N^{-1}[\underline{X}'\underline{X}]$ is a matrix of moments of the design. For example, if there were $k = 2$ variables, and we were considering a design of order two so that the equation to be fitted was

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

then

$$N^{-1}[\underline{X}'\underline{X}] = \begin{array}{c} 0 \\ 1 \\ 2 \\ 11 \\ 22 \\ 12 \end{array} \begin{bmatrix} 1 & [1] & [2] & [11] & [22] & [12] \\ [1] & [11] & [12] & [111] & [122] & [112] \\ [2] & [12] & [22] & [112] & [222] & [122] \\ [11] & [111] & [112] & [1111] & [1122] & [1112] \\ [22] & [122] & [222] & [1122] & [2222] & [1222] \\ [12] & [112] & [122] & [1112] & [1222] & [1122] \end{bmatrix} \tag{10}$$

where 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. It will be noted that in a fitted expression of the form of (4), in which terms of order greater than the first are included, many of the independent variables are related to each other, thus we have not only x_1, but x_1^2, and $x_1 x_2$ occuring in equation (9). Consider for a moment an expression of the form

$$\eta = \beta_0 z_0 + \beta_1 z_1 + \beta_2 z_2 + \ldots + \beta_L z_L \tag{11}$$

and suppose the sum of squares for the p^{th} variable $\sum_{u=1}^{N} z_{pu}^2$ is denoted by S_p. Then it is readily shown, (see for example Box 1952) that if the S_p are regarded as fixed the smallest possible variance for every one of the elements b_0, b_1, etc. is obtained if the moment matrix and hence of course the precision matrix are diagonal, assuming that such a diagonal form is possible. In such a case the variance of the p^{th} effect is given by $S_p^{-1}\sigma^2$. In the case of first order designs in which the terms in (11) are unrelated this fact supplies the necessary conditions for an optimal design. To satisfy the condition we chose the levels $z_0, z_1, \ldots, z_L$ so that the L vectors formed by the columns of the matrix of independent variables have zero inner products one with another.

When fitting an equation of degree higher than the first, provided $\underline{X}$ is of full rank L, we may still, of course, use the procedure of least squares to estimate the effects even though the independent variables are related to one another. However, when an equation of degree greater than the first is fitted, these relationships make impossible the attainment of a diagonal matrix for $\underline{X}'\underline{X}$. For example, both [11], [22] which appear in non-diagonal positions in (10) must of necessity be positive unless all the x_{iu} are to be zero. In general $\sum_{u=1}^{N} x_{iu}^p\, x_{iu}^q$ will produce essentially non-zero elements where p plus q is an even number, and these terms can occur in non-diagonal positions when $p \neq q$. We can however rewrite equation (4) in terms of new variables $x^{\bar{2}}$, $x^{\bar{3}}$, $x^{\bar{4}}$, which are $\left\{\begin{matrix}\text{odd}\\ \text{even}\end{matrix}\right\}$ polynomials $x^{\bar{p}} = x^p - \alpha_1 x^{p-2} - \alpha_2 x^{p-4}$ etc. orthogonal to all other $\left\{\begin{matrix}\text{odd}\\ \text{even}\end{matrix}\right\}$ powers of lower degree and

$$\sum_{u=1}^{N} x_{iu}^{\overline{p-2r}}\; x_{iu}^{\bar{p}} = 0 \qquad (12)$$

where r is an integer. For example we require

$$\sum_{u=1}^{N} x_{iu}^{\bar{2}} = \sum_{u=1}^{N} (x_{iu}^2 - \alpha) = 0 \qquad (13)$$

whence using (3) $\alpha = 1$ and $\bar{x}_i^2 = x_{iu}^2 - 1$ (14)

Similarly $x_i^3 = x_i^3 - [iiii]\, x_i$ (15)

The equations written in terms of these new variables would be

$$\eta = (\underline{X}\underline{T})(\underline{T}^{-1}\underline{\beta}) = \dot{\underline{X}}\,\dot{\underline{\beta}} \qquad (16)$$

where $\underline{T}$ is a matrix transforming the old independent variables to the new, thus in terms of the new variables (9) could be written in the form

$$\eta = (\beta_0 + \beta_{11} + \beta_{22})x_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11}(x_1^2 - 1) + \beta_{22}(x_2^2 - 1) + \beta_{12}x_1x_2 \qquad (17)$$

and
$$\underline{T} = \begin{bmatrix} 1 & \cdot & \cdot & -1 & -1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ -1 & \cdot & \cdot & 1 & \cdot & \cdot \\ -1 & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{bmatrix} \qquad \underline{T}^{-1} = \begin{bmatrix} 1 & \cdot & \cdot & 1 & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & 1 & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & 1 \end{bmatrix} \qquad (18)$$

replace by a dot

replace by a dot

For the new independent variables it is now possible to attain an orthogonal matrix for any permissable choice of diagonal elements. The Gauss-Markoff theorem, (Guass, 1831, Markoff, 1912,) ensures that the least squares estimates obtained for these new variables will also be least squares estimates for the old variables.

We have agreed to define the elements in the design matrix so that

$\sum_{u=1}^{N} x_{ou}^2 = N$, and $\sum_{u=1}^{N} x_{iu}^2 = N$ $(i = 1,2,\ldots,k)$, therefore, the first $k + 1$ diagonal elements of the matrix $\underline{X}'\underline{X}$ will be fixed and equal to N. The remaining diagonal elements of $\underline{X}'\underline{X}$ will not be fixed by our definition. For example, it is easy to show that the sum of squares $\sum_{u=1}^{N} (x_{iu}^2 - 1)^2$ corresponding to the i^{th} quadratic variable can take any value between zero and $N(N-2)^2/(N-1)$. This is what is meant by a "permissable" choice of diagonal elements. The remaining sums of squares would likewise be at our choice within certain wide ranges.

Consider the case of a design of order two. The choice of the quantity $N^{-1}\sum_{u=1}^{N}(x_{iu}^2-1)^2 = q = [iiii] - 1$ corresponds to the choice of the fourth moment for the i^{th} variable in the design, that is, of a fourth marginal moment of the distribution of design points. Since $[ii] = 1$, $[iiii] - 3$ is the measure of kurtosis γ_2, the standardized fourth cumulant of the marginal distribution and $q = \gamma_2 + 2$. Suppose we fix q at some particular value, then for example with $k = 2$ factors, the design will be such that the moment matrix for the orthogonal variables will be

$$N^{-1}[\dot{\underline{X}}'\dot{\underline{X}}] = \begin{bmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ & 1 & \cdot & \cdot & \cdot & \cdot \\ & & 1 & \cdot & \cdot & \cdot \\ & & & q & \cdot & \cdot \\ & & & & q & \cdot \\ & & & & & 1 \end{bmatrix} ; \quad N^{-1}[X'X] = \begin{bmatrix} 1 & \cdot & \cdot & 1 & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & q+1 & 1 & \cdot \\ 1 & \cdot & \cdot & 1 & q+1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{bmatrix} \qquad (19)$$

The diagonal element in $N^{-1}[\underline{X}'\underline{X}]$ corresponding to the interaction term $[1122]$ is fixed automatically, since to ensure orthogonality of the quadratic effects

$$N^{-1}\sum^{N}(x_{iu}^2-1)(x_{2u}^2-1) = [1122] - [11] - [22] + 1 = [1122] - 1 = 0$$

Hence $[1122] = 1$. The corresponding moment matrix $N^{-1}(\underline{X}'\underline{X})$ for $d = 2$ and any value of k will be exactly similar in pattern, that is to say, the element $[ii]$

corresponding to the sum of squares of the i^{th} linear variable and the sum of products between x_0 and the i^{th} quadratic variable will always be equal to one. The element $[iiii]$ corresponding to the i^{th} quadratic effect will always be equal to $q + 1$ and the element $[iijj]$ corresponding to the sum of products between the i^{th} and j^{th} quadratic variable, and to the sum of squares of the ij^{th} interaction variable will be unity. All other elements are zero. Similarly, the variance-covariance matrix written on a "per-observation" basis would be

$$N[\dot{X}'\dot{X}]^{-1} = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & q^{-1} & & \\ & & & & q^{-1} & \\ & & & & & 1 \end{bmatrix}$$ and for the original non-orthogonal variables $$N[X'X]^{-1} = \begin{bmatrix} 1+kq^{-1} & \cdot & \cdot & -q^{-1} & -q^{-1} & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ -q^{-1} & \cdot & \cdot & q^{-1} & \cdot & \cdot \\ -q^{-1} & \cdot & \cdot & \cdot & q^{-1} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{bmatrix}$$

For the 3^2 factorial (and in general for the 3^p factorial design) $q = 1/2$ that is $\gamma_2 = -\frac{3}{2}$. Thus, using these designs, the variance of the quadratic effects is twice that for the interaction effect(s). As was pointed out in an earlier paper, (Box and Wilson, 1951, pg. 18) if we regard (9) as representing a Taylor's Series of the function $\eta = f(x_1 x_2)$ then $\beta_{11} = \frac{1}{2}\varphi_{11}$; $\beta_{22} = \frac{1}{2}\varphi_{22}$; $\beta_{12} = \varphi_{12}$ where for example $\varphi_{12} = \partial^2\eta/\partial x_1 \partial x_2$. Thus the variance of the quadratic <u>derivatives</u> is eight times that of the interaction derivatives. This relative weighting for quadratic and interaction terms found for the factorial design seems intuitively to be unsatisfactory from the point of view of accurate estimation of the fitted surface, for it appears that too little weight is placed on the quadratic terms as compared to the interaction terms. This fact may be the reason for a mis-conception concerning the relative importance of quadratic and interaction effects. It is commonly found in the analysis of variance of three level factorial designs that two-factor interactions are significant whereas quadratic effects are not. This has led to a supposition that conditions frequently occur in which two-factor interactions are important but quadratic effects are unimportant, which apparently conflicts with the common sense view that for a smooth surface effects of the same order ought to be of equal importance. That this contradiction is apparent rather than real can be seen if we remember that these expected values of the mean squares in the analysis of variance are of the form

$$\sigma^2 + \beta^2 \Big/ \frac{V(b)}{\sigma^2} \qquad (21)$$

It will be noted that the second term in (21), which will cause the mean square to be inflated when real effects occur, is a function not only of the size of the effect β but also of the variance of the estimate of this quantity. Thus if real quadratic and interaction derivatives of equal magnitude occured the inflation of the mean squares for the interaction would be eight times as large on the average as the inflation of the mean squares for the quadratic effects.

When $d = 3$ we have the cubic design in which all effects up to order three are estimated. When $k = 2$ the equation $\eta = \underline{X\beta}$ to be fitted is

$$\eta = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \beta_{111} x_1^3 + \beta_{222} x_2^3 + \beta_{112} x_1^2 x_2 + \beta_{122} x_1 x_2^2 \qquad (22)$$

which, proceeding as before, may be written in the alternative form

$$\eta = [\underline{X}\ \underline{T}][T^{-1}\beta]$$

$$\eta = (\beta_0 + \beta_{11} + \beta_{22})x_0 + \left\{\beta_1 + (q+1)\beta_{111} + \beta_{122}\right\} x_1 + \left\{\beta_2 + (q+1)\beta_{222} + \beta_{112}\right\} x_2 + \beta_{11}(x_1^2 - 1) + \beta_{12}(x_2^2 - 1)$$
$$+ \beta_{12} x_1 x_2 + \beta_{111}\left\{x_1^3 - (q+1)x_1\right\} + \beta_{222}\left\{x_2^3 - (q+1)x_2\right\} + \beta_{112}(x_1^2 - 1)x_2 + \beta_{122} x_1 (x_2^2 - 1) \qquad (23)$$

We may now introduce a further parameter

$$r = N^{-1}\sum_{u=1}^{N}\left\{x_{iu}^{3} - (q+1)x_{iu}\right\}^{2} = \gamma_4 - \gamma_2^2 + 9\gamma_2 + 6$$

where

$$\gamma_4 = \frac{K_6}{K_2^3} = \frac{\mu_6 - 15\mu_4\mu_2 - 10\mu_3^2 + 30\mu_2^2}{\mu_2^3}$$

$$\gamma_4 = \mu_6 - 15\mu_4 + 30$$

Proceeding as before we have

$$N^{-1}[X'X] = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 11 \\ 22 \\ 12 \\ 111 \\ 222 \\ 112 \\ 122 \end{array}\begin{array}{c} \begin{array}{cccccccccc} 0 & 1 & 2 & 11 & 22 & 12 & 111 & 222 & 112 & 122 \end{array} \\ \left[\begin{array}{cccccccccc} 1 & & & & & & & & & \\ & 1 & & & & & & & & \\ & & 1 & & & & & & & \\ & & & q & & & & & & \\ & & & & q & & & & & \\ & & & & & 1 & & & & \\ & & & & & & r & & & \\ & & & & & & & r & & \\ & & & & & & & & q & \\ & & & & & & & & & q \end{array}\right] \end{array} \qquad (24)$$

where the diagonal terms corresponding to the quadratic x linear interactions are necessarily fixed by the orthogonality conditions. For we require that

$$N^{-1}\sum_{u=1}^{N}\left\{x_{iu}^{3}-(q+1)x_{iu}\right\}\left\{x_{iu}x_{ju}^{2}-x_{iu}\right\} = [iiiijj]-(q+1) = 0, \text{ i.e., } [iiiijj] = q + 1$$

But

$$N^{-1}\sum_{u=1}^{N}\left\{(x_{iu}^{2} - 1)x_{ju}\right\}^{2} = [iiiijj] - 1 = q.$$

Proceeding as before, the moment matrix $N^{-1}[\underline{X}'\underline{X}]$ for the original variables is $= N^{-1}(T^{-1})'\dot{X}'\dot{X}T^{-1}$

$N^{-1}[\bar{X}'X]$

$= N^{-1}\underline{T}^{-1}{}'\dot{\underline{X}}'\dot{\underline{X}}\underline{T}^{-1}$

$$
\begin{array}{cccccccccc}
0 & 1 & 2 & 11 & 22 & 12 & 111 & 222 & 112 & 122 \\
1 & & & 1 & 1 & & & & & \\
 & 1 & & & & & q+1 & & & 1 \\
 & & 1 & & & & & q+1 & 1 & \\
1 & & & q+1 & 1 & & & & & \\
1 & & & 1 & q+1 & & & & & \\
 & & & & & 1 & & & & \\
 & q+1 & & & & & r+(q+1)^2 & & & q+1 \\
 & & q+1 & & & & & r+(q+1)^2 & q+1 & \\
 & & 1 & & & & & q+1 & q+1 & \\
 & 1 & & & & & q+1 & & & q+1
\end{array}
$$

N times the precision matrix $N[X'X]^{-1}$ for the original variables is

$N\underline{T}[\dot{\underline{X}}'\dot{\underline{X}}]^{-1}\underline{T}' =$

$$
\begin{array}{c}
\begin{array}{cccccccccc}
0 & 1 & 2 & 11 & 22 & 12 & 111 & 222 & 112 & 122
\end{array} \\
\left[\begin{array}{cccccccccc}
1+2q^{-1} & & & -q^{-1} & -q^{-1} & & & & & \\
 & 1+(q+1)^2r^{-1}+q^{-1} & & & & & -(q+1)r^{-1} & & & -q^{-1} \\
 & & 1+(q+1)^2r^{-1}+q^{-1} & & & & & -(q+1)r^{-1} & -q^{-1} & \\
-q^{-1} & & & q^{-1} & & & & & & \\
-q^{-1} & & & & q^{-1} & & & & & \\
 & & & & & 1 & & & & \\
 & -(q+1)r^{-1} & & & & & r^{-1} & & & \\
 & & -(q+1)r^{-1} & & & & & -r^{-1} & & \\
 & & -q^{-1} & & & & & & q^{-1} & \\
 & -q^{-1} & & & & & & & & q^{-1}
\end{array}\right]
\end{array}
$$

2.778 0.64 0.2304

For the four level factorial, for example, $q = 1.62$ and $r = 0.2996$ thus $q/r = 5.407$, so that in this design, the variance of the cubic effects b_{iii} is 5.407 times as large as that for the quadratic times linear interaction b_{ijj}. In terms of derivatives the variance of φ_{iii} is over 48 times as large as that for φ_{iij}.

3. DEPENDENCE OF THE PROPERTIES OF DESIGNS ON THEIR ORIENTATION

Whereas, with the designs of order one, the principal of minimizing the variance of the effects for a given spread of the design points leads to the criterion of orthogonality (which gives uniquely a simple class of designs), for designs of order greater than one this principal does not lead to such a unique class. If we decide what the relative variance of the effects should be, and hence what the diagonal elements of the moment matrix will be, we may, by using an orthogonal design, obtain smallest possible variance for this choice of diagonal elements. However this approach gives no clue as to <u>what</u> values for the diagonal elements we should choose. Some further principal is required to make such a decision. Now we wish to use the designs to explore a local response surface of which little is known. It particular the orientation of the surface with respect to the design is unknown. 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 principle axes. The orientation of these axes and the direction of the center of the system relative to the axes of the factors would differ from one problem to another. In these circumstances it would seem unsatisfactory if the accuracy with which the constants of the surface were estimated depended on the orientation of these axes.

3.1 EFFECT OF ROTATING AN ORTHOGONAL DESIGN

In the developments which follow we need to use some properties of derived power and product vectors and the corresponding Schläflian matrices (Aitken; 1948, 1949, Wedderburn; 1934). If $\underline{x}' = (x_1, x_2, \ldots, x_k)$ then we denote by $x'^{[p]}$ the derived power vector of degree p. For example if $k = 2$

$$\underline{x}' = [x_1, x_2] \text{ and } \underline{x}'^{[2]} = [x_1^2,\ x_2^2,\ \sqrt{2}x_1x_2]$$

and in general $\underline{x}'^{[p]}$ will contain as elements all the powers and products of degree p and less ~~duly orders of the elements in x'~~ with suitable multipliers attached so that $\underline{x}'^{[p]}\,\underline{x}^{[p]} = [\underline{x}'\,\underline{x}]^{[p]}$. If a vector $\underline{x}$ is transformed to a vector $\underline{z}$ by $\underline{z} = \underline{H}\,\underline{x}$, the p^{th} Schläflian matrix $\underline{H}^{[p]}$ is defined such that $\underline{z}^{[p]} = \underline{H}^{[p]}\underline{x}^{[p]}$. It is readily confirmed that $[\underline{H}\,\underline{k}]^{[p]} = \underline{H}^{[p]}\,\underline{k}^{[p]}$. Also if H is orthogonal then so also is $\underline{H}^{[p]}$.

We may now consider the effect of rotating an orthogonal design. Consider in particular the case $k = 2$, $d = 2$, and let us write the equation to be fitted in the form $\eta = \underline{x}\,\underline{\beta}$, that is

$$\eta = (\beta_0 + \beta_{11} + \beta_{22})x_0 + \beta_1x_1 + \beta_2x_2 + \beta_{11}(x_1^2 - 1) + \beta_{22}(x_2^2 - 1) + \frac{1}{\sqrt{2}}\beta_{12}\sqrt{2}x_1x_2 \quad (27)$$

Suppose we have selected some orthogonal arrangement for which the design matrix is $\underline{D}$ and $q = \gamma_2 + 2$ has some specific value. The matrix $N^{-1}[\underline{X}'\underline{X}]$ is then

$$N^{-1}[\underline{X}'\underline{X}] = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 11 \\ 22 \\ 12 \end{array}\begin{array}{c} \begin{array}{cccccc} 0 & 1 & 2 & 11 & 22 & 12 \end{array} \\ \left[\begin{array}{cccccc} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 2+\gamma_2 & & \\ & & & & 2+\gamma_2 & \\ & & & & & 2 \end{array}\right] \end{array} \quad (28)$$

If the design is orthogonallly rotated through an angle θ so that the new design matrix is $\dot{\underline{D}} = \underline{D}\,\underline{H}$ and $H = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$ where s is sine θ and c is consine cosine θ, then the u^{th} row vector in $\underline{D}$, $\underline{x}'_u = [x_{1u}, x_{2u}]$ will be transformed to a new row vector $\underline{w}_u$ by the transformation $\underline{w}'_u = \underline{H}\,\underline{x}'_u$. The transformation which carries over $\underline{x}'^{[2]}_u = [x^2_{1u},\ x^2_{2u},\ \sqrt{2}x_{1u}\,x_{2u}]$ to $\underline{w}'^{[2]}_u = [w^2_{1u}, w^2_{2u}, \sqrt{2}w_{1u}\,w_{2u}]$ is

$$\underline{H}^{[2]} = \begin{bmatrix} c^2 & s^2 & -sc\sqrt{2} \\ s^2 & c^2 & sc\sqrt{2} \\ sc\sqrt{2} & -sc\sqrt{2} & c^2 - s^2 \end{bmatrix}$$

This transformation likewise carries over the modified vector

$[x^2_{1u} - 1,\ x^2_{2u} - 1,\ \sqrt{2}x_{1u}x_{2u}]$ to the modified vector

$[w^2_{1u} - 1,\ w^2_{2u} - 1,\ \sqrt{2}w_{1u}w_{2u}]$; for the vector (1, 1, 0) is always a latent vector of $\underline{H}^{[2]}$.

After rotating, the 3 x 3 matrix $\underline{P}$ in the lower right hand corner of the transformed moment matrix becomes

$$\dot{\underline{P}} = \underline{H}'^{[2]} \left\{ (2+\gamma_2)\underline{I}_3 - \begin{bmatrix} 0 & & \\ & 0 & \\ & & \gamma_2 \end{bmatrix} \right\} \underline{H}^{[2]} \qquad (30)$$

$$= (2+\gamma_2)\underline{I}_3 - \gamma_2\underline{a}\,\underline{a}' = (2+\gamma_2)\left\{ \underline{I} - \frac{\gamma_2}{2+\gamma_2}\,\underline{a}\,\underline{a}' \right\} \qquad (31)$$

where $\underline{a}$ is the 3 x 1 vector with elements omit $-$ $sc\sqrt{2}, -sc\sqrt{2}, c^2 - s^2$. In general this matrix $\dot{\underline{P}}$ will contain off-diagonal terms. Its reciprocal may be readily found using a formula given by Tochar (1951), who shows that $(\underline{I} + \underline{ML})^{-1} = \underline{I} - \underline{M}(\underline{I} - \underline{LM})^{-1}\,\underline{L}$. Where $\underline{L}$ and $\underline{M}$ are not necessarily square matrices. Putting $\frac{-\gamma_2}{(2+\gamma_2)}\,\underline{a} = \underline{M}$ and $\underline{a}' = \underline{L}$

we obtain

$$\frac{\gamma_2}{2(\gamma_2+1)}$$

$$\underline{P}^{-1} = (\gamma_2 + 2)^{-1} \left\{ \underline{I} + \frac{1}{2}\gamma \, \underline{a} \, \underline{a}' \right\} \tag{32}$$

From elementary trigonometry $\underline{a}\,\underline{a}'$ may be expressed in terms of cos 4θ and cos 8θ only (written as c_4 and c_8) and finally we obtain

$$\underline{P}^{-1} = (\gamma_2 + 2)^{-1} \left\{ \underline{I} + \frac{1}{8}\gamma \begin{bmatrix} A & -A & +B \\ -A & A & -B \\ +B & -B & C \end{bmatrix} \right\} \tag{33}$$

where $A = \frac{1}{4}(1 - c_4)$, $B = \frac{1}{2\sqrt{2}} s_4$, and $C = \frac{1}{2}(1 + c_4)$. The matrix $N\underline{C}^{-1}$ is therefore

$$N[\tilde{\underline{X}}'\tilde{\underline{X}}]^{-1} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & P^{-1} \end{bmatrix} \tag{34}$$

The linear effects have the same variance in all orientations and are uncorrelated with all other terms. However for second order terms the variances change markedly as the design is rotated and the effects become correlated.

As an example, the effect of rotation on the variances and correlations of the second order effects in the three level factorial design is shown in Table 2 and illustrated in Figure 1.

Angle of Rotation θ	0°	15°	22.5°	30°	45°
Variance Quadratics	2	1.8	1.63	1.44	1.25
Variance Interaction	1	1.75	2.50	3.25	4.00
Correlation Quadratic x Quadratic	0	0.10	0.23	0.39	0.60
Correlation Quadratic x Interaction	0	-0.32	-0.37	-0.26	0

Table 2: Change in Standardized Variances $N\,V(b)/\sigma^2$ of Effects as Factorial Design is Rotated.

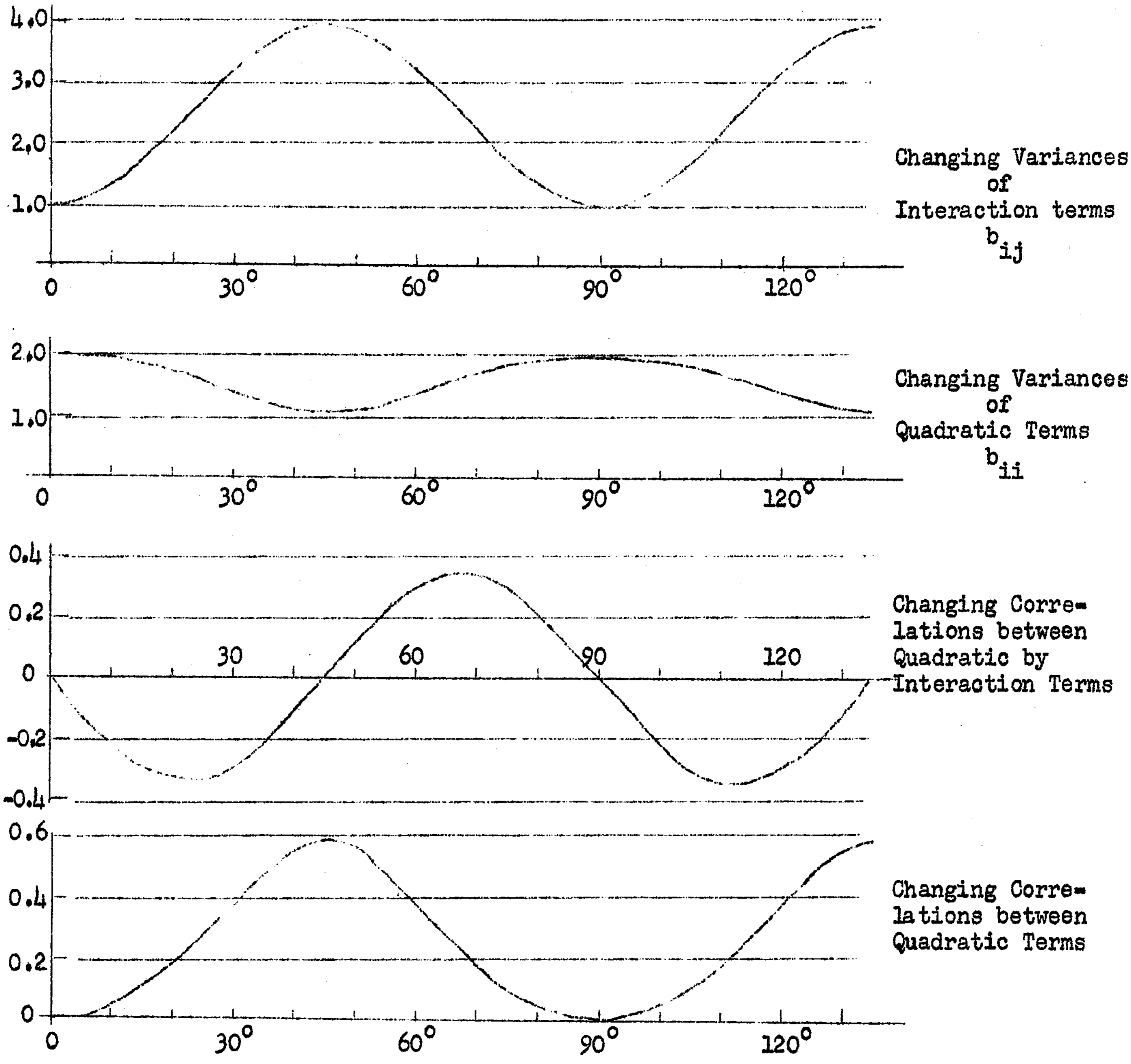


Figure 1

3^2 Factorial Design Under Rotation Standardized Variances of Effects

We see that our condition of orthogonality refers to orthogonality in a particular orientation and that this property will usually be lost on rotation of the design. We notice also that since the variance and covariance of the effects may change markedly from one orientation to another, the apparent efficiency of the design, as judged by inspection of the variances in one particular orientation, may be deceptive.

4. INFORMATION DISTRIBUTIONS

The object of our experimentation is to gain knowledge of a response surface which it is assumed may be represented by an equation of a certain form. We are interested in the individual terms in the equation and their variances only in so far as they supply us information about this surface.

Suppose that some surface had been fitted. The predicted response $\dot{y}$ at a given point $x_1, x_2, \ldots, x_k$ would be provided by the equation

$$\dot{y} = \theta(x_1, x_2, \ldots, x_k) \tag{35}$$

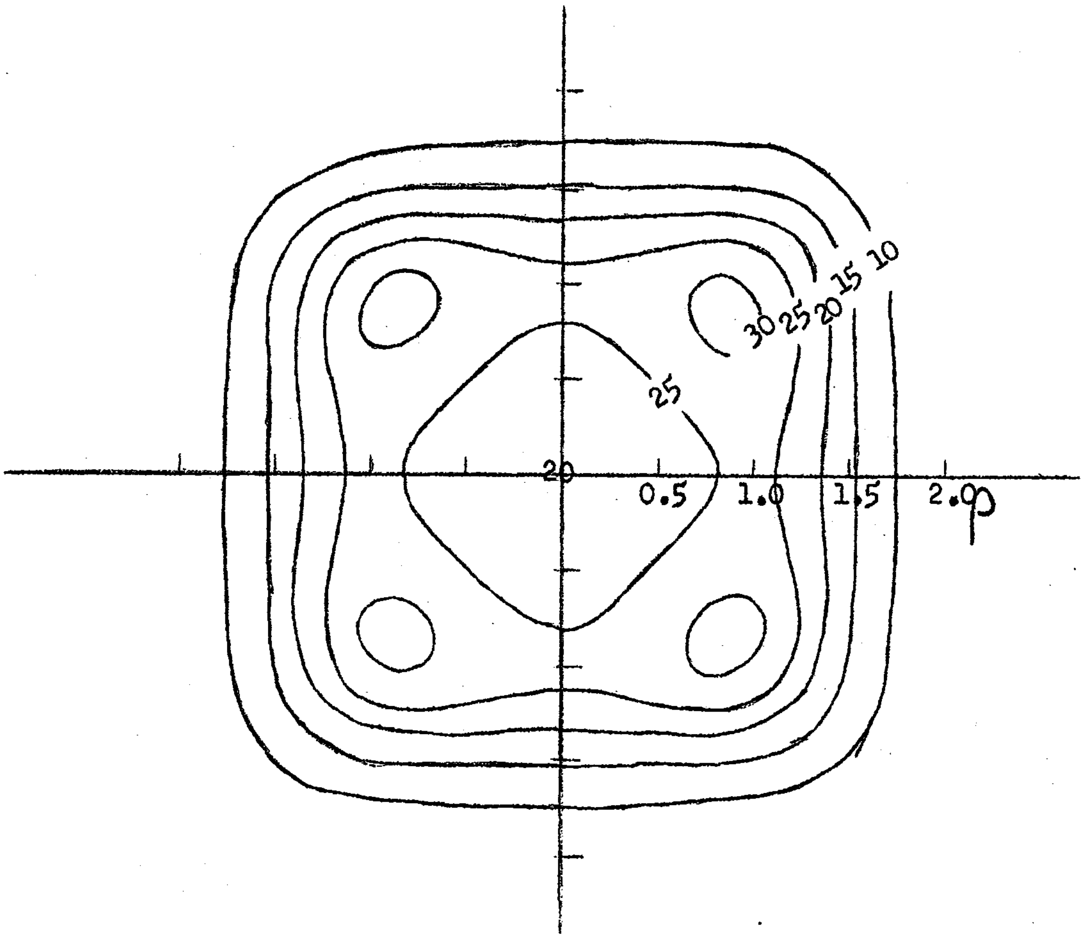
The variance of this predicted value would also be a function of $x_1, x_2, \ldots, x_k$ and hence so would the distribution of information in the space of the factors. Writing $I(y)$ for the information per observation we have

$$I(y) = \left\{NV(y)\right\}^{-1} = \xi(x_1, x_2, \ldots, x_k) \tag{36}$$

where $\xi(x_1, x_2, \ldots, x_k)$ may be called the information distribution. For example using the three level factorial design in the case $d = 2$, $k = 2$, we see from equation (19) that the information distribution is

$$I(y) = \left[5 - 3x_1^2 - 3x_2^2 + 2x_1^4 + 2x_2^4 + x_1^2x_2^2\right]^{-1} \Big/ \sigma^2 \tag{37}$$

Information contours for this distribution are shown in Figure 3.



ρ = distance out from center of design

Figure 3

Contours of Information Distribution for 3^2
Factorial Design Assuming a Second Degree Equation

as would be expected from the earlier discussion and indeed from the placement of the points we see that at a given distance from the origin a greater concentration of information exists in some directions than in others.

It seems of some importance to consider designs, if such exist, which have the property that the information is constant at a given distance from the origin, in other words, the information contours are circles, spheres or hyperspheres. Such arrangements will be called rotatable designs.

5. CONDITIONS FOR ROTATABILITY

We shall need to consider some properties of spherical distribution functions, (Box 1953). These distribution functions are of some importance in basic statistical theory, and especially in randomization theory. A discussion of these aspects is left to a later publication. Here we shall need them for a somewhat different purpose.

If the joint distribution function of a set of variates, $z_1, z_2, \ldots, z_k$, which may be regarded as the elements of a vector $\underline{z}$, and each of which has zero mean and unit variance, can be written in the form

$$p(\underline{z}) = kf(\underline{z}'\underline{z}) \qquad 0 \leq \underline{z}'\underline{z} < \overset{W}{\omega} \qquad (38)$$

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 variates have a spherical distribution.

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

$$\varphi(t) = 1 + \sum_{S=1}^{\infty} \frac{1}{S!} t'^{[S]} \underline{m}_S \qquad (39)$$

then it has been shown, (J. Clarke Maxwell, 1820, M. S. Bartlett, 1934) 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

$$\varphi(t) = \exp \frac{1}{2} (\underline{t}'\underline{t}) \tag{45}$$

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. However the moments of different orders will depend on the λ's and hence on the function $f(\underline{z}'\underline{z})$.

Consider the response $\dot{y}$ predicted by the regression equation at the particular point whose co-ordinates are given by the last k elements of the vector $\underline{x}'$ now defined as $\underline{x}' = (1, x_1, x_2, \ldots, x_k)$. Since the equation fitted is a polynomial in the k factors of degree d then the polynomial contains $\binom{k+d}{k} = L$ terms and the fitted equation

$$\dot{y} = b_0 + b_1x_1 + b_2x_2 + \ldots + b_kx_k + b_{11}x_1^2 + b_{22}x_2^2 + \ldots + b_{kk}x_k^2 + b_{12}x_1x_2 + \ldots + b_{k-1,k}x_{k-1}x_k \tag{46}$$

may be written

$$\dot{y} = \underline{x}'^{[d]}\underline{b} \quad \text{(note } \dot{y} \text{ is a single predicted value.)} \tag{47}$$

where the L x 1 vector $\underline{b}$ contains all the b's with suitable multipliers attached so that (47) is equivalent to (46). Suppose also that the true value at this point is given by

$$\eta = \underline{x}'^{[d]}\underline{\beta} \quad \text{(a scalar)} \tag{48}$$

Then the variance of this predicted value is

$$V(\hat{y}) = \mathcal{E}(y-\eta)(y-\eta)' = \underline{x}'^{[\bar{d}]}\mathcal{E}(\underline{b}-\underline{\beta})(\underline{b}-\underline{\beta})'\,\underline{x}^{[\bar{d}]} = \underline{x}'^{[d]}[\underline{X}'\underline{X}]^{-1}\underline{x}^{[\bar{d}]}\,\sigma^2 \tag{49}$$

The variance at a second point which is the same distance ρ from the origin whose co-ordinates are the last k elements of the vector $\underline{z} = \underline{R}\,\underline{x}$ where $\underline{R}$ is an orthogonal $(k + 1) \times (k + 1)$ matrix consisting of an arbitrary orthogonal matrix $\underline{H}$ bordered by a first row $\underline{u}' = (1, 0, 0, \ldots, 0)$ and a first column $\underline{u}$. Making the substitution in (49) we have

$$V(\hat{y}) = x'^{[\bar{d}]}R'^{[\bar{d}]}\,[\underline{X}'\underline{X}]^{-1}\,R^{[\bar{d}]}x^{[\bar{d}]} \tag{50}$$

$$= x'^{[\bar{d}]}\,(R'^{[\bar{d}]}\underline{X}'\underline{X}\;R^{[\bar{d}]})^{-1}\,x^{[\bar{d}]} \tag{51}$$

To satisfy the condition that the variance is constant on a sphere centered at the origin of the design we require therefore that the precision matrix $C^{-1} = [\underline{X}'\underline{X}]^{-1}$, and hence also the moment matrix $N^{-1}\underline{C} = N^{-1}\underline{X}'\underline{X}$, remain invarient when the design is rotated. This means of course that every variance and covariance of the b's and all the moments and mixed moments of the design remain constant under rotation.

We now have to find the form of the matrices $\underline{C}$ and $\underline{C}^{-1}$ for which this is so. Consider the quadratic form

$$Q = (N^{-1})\underline{t}'^{[\bar{d}]}\;\underline{C}\;\underline{t}^{[\bar{d}]} \tag{52}$$

Q is a generating function for the moments of order 2d and less of the design, for

$$Q = N^{-1}\underline{t}'^{[\bar{d}]}\sum_{u=1}^{N}x_u^{[\bar{d}]}\,x_u'^{[\bar{d}]}\underline{t}^{[\bar{d}]} = N^{-1}\sum_{u=1}^{N}(\underline{t}'\underline{x}_u\underline{x}_u'\underline{t})^d \tag{53}$$

$$= N^{-1}\sum_{u=1}^{N}\left(1 + t_1x_{1u} + t_2x_{2u} + \cdots + t_kx_{ku}\right)^{2d} \tag{54}$$

where $\underline{m}_S$ is the vector of moments $\mathcal{E}\{x^{[S]}\}$. But for a spherical distribution the m.g.f. is

$$\varphi(t) = \mathcal{E}(e^{\underline{t}'\underline{z}}) = \mathcal{E}(e^{\underline{t}'\underline{H}\,\underline{z}}) \tag{40}$$

$$\text{i.e.}\quad \varphi(\underline{t}) = \varphi(\underline{H}\,\underline{t})$$

for any orthogonal matrix $\underline{H}$. Regarding now the matrix $\underline{H}$ as transforming the matrix $\underline{t}'$ this implies that $\varphi(t)$ is unchanged by any transformation on $\underline{t}$ which leaves $\underline{t}'\underline{t}$ unchanged. This m.g.f. is then a function of $\underline{t}'\underline{t}$

$$\varphi(t) = 1 + \sum_{p=1}^{\infty} \omega_{2p}(t't)^p \tag{41}$$

where the ω_S' are real constants depending on the function f in (38). Writing $\lambda_{2p} = W_{2p}(p!)2^p$ the m.g.f. for the spherical distribution can be written in this form

λ_{2p}

$$\varphi(t) = 1 + \sum_{p=1}^{\infty} \omega_{2p} \frac{1}{p!\,2^p}(\underline{t}'\underline{t})^p \tag{42}$$

Equating terms in (39) and (42) and writing $[1^{\alpha_1}, 2^{\alpha_2}, \dots, k^{\alpha_k}]$ for the moment $\mathcal{E}[x_1^{\alpha_1}, x_2^{\alpha_2}, \dots, x^{\alpha_k}]$ we have

$$[1^{\alpha_1}, 2^{\alpha_2}, \dots, k^{\alpha_k}] = \lambda_\alpha \frac{\prod_{i=1}^{k} \alpha_i!}{2^{\alpha/2}\prod_{i=1}^{k}(\frac{1}{2}\alpha_i)!} \tag{43}$$

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

If the z's are independent so that

$$p(z) = \prod_{i=1}^{k} p(z_i) \tag{44}$$

and the coefficient of $t_1^{\alpha_1}, t_2^{\alpha_2}, \ldots, t_k^{\alpha_k}$, in this expression is

$$\frac{2d!}{\alpha_1!\,\alpha_2!\,\ldots\,\alpha_k!\,(2d-\alpha)!}[1^{\alpha_1}, 2^{\alpha_2}, \ldots, k^{\alpha_k}] \tag{55}$$

where $[1^{\alpha_1}, 2^{\alpha_2}, \ldots, k^{\alpha_k}]$ is the moment $N^{-1}\sum_{u=1}^{N}(x_{1u}^{\alpha_1}, x_{2u}^{\alpha_2}, \ldots, x_{ku}^{\alpha_u})$ (56)

Now we require that $\underline{C}$ should be such that

$$Q = N^{-1}\underline{t}'^{[d]}\underline{C}\,\underline{t}^{[d]} = N^{-1}\underline{t}'^{[d]}\underline{R}'^{[d]}\underline{C}\,\underline{R}^{[d]}\underline{t}^{[d]} \tag{57}$$

$$Q = N^{-1}(\underline{t}'\underline{R}')^{[d]}\,\underline{C}\,(\underline{R}\,\underline{t})^{[d]} \tag{58}$$

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

$$Q = \sum_{S=0}^{d} a_{2S}\left(\sum_{i=1}^{k} t_i^2\right)^S \tag{59}$$

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

$$a_\alpha \cdot \frac{(\frac{1}{2}\alpha)!}{(\frac{1}{2}\alpha_1)!\,(\frac{1}{2}\alpha_2)!\,\ldots\,(\frac{1}{2}\alpha_k)!} \tag{60}$$

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

$$[1^{\alpha_1}, 2^{\alpha_2}, \ldots, k^{\alpha_k}] = \frac{a_\alpha(\frac{1}{2}\alpha)!\,(2d-\alpha)!}{2d!} \cdot \frac{\prod_{i=1}^{k}\alpha_i!}{\prod_{i=1}^{k}(\frac{1}{2}\alpha_i)!} \tag{61}$$

Write

$$\frac{a_\alpha 2^{\frac{1}{2}\alpha} (\frac{1}{2}\alpha)! \, (2d - \alpha)!}{2d!} = \lambda_\alpha \qquad (62)$$

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

$$[1^{\alpha_1}, 2^{\alpha_2}, \ldots, k^{\alpha_k}] = \begin{cases} 0 & \text{if one or more of the } \alpha_i \text{ are odd} \\ \lambda_\alpha \dfrac{\prod_{i=1}^{k} \alpha_i!}{2^{1/2\alpha} \prod_{i=1}^{k} (\frac{1}{2}\alpha_i)!} & \text{if all of the } \alpha_i \text{ are even} \end{cases} \qquad (63)$$

which (in equation (43)) are the moments up to order 2d of the spherical distribution.

Thus a design of order d will have the property that when a polynomial of degree d in the variables $x_1, x_2, \ldots, x_k$ is fitted by the method of least squares all points at the same distance ρ from the origin of the design are estimated with equal accuracy if and only if the moments of the design up to order 2d are those of a spherical distribution. That is, those given by equation (43) where the λ's are arbitrary. With these values the information distribution will be spherical and as we have seen, the moments of the design and the variances and covariances will remain constant whatever its orientation.

Since the dummy variable x_0 is always unity, and we have selected the design so that $N^{-1} \sum_{u=1}^{N} x_{iu}^2 = 1$, λ_0 and λ_2 are such equal to unity by assumption.

5.1 ROTATABLE DESIGNS OF ORDER 1

Suppose we have k variables $x_1, x_2, \ldots, x_k$ and we fit a polynomial of degree $d = 1$, that is to say the fitted equation represents a plane,

$$\hat{y} = b_0 + b_1x_1 + b_2x_2 + \ldots + b_kx_k \qquad (64)$$

then using (63)

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

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

quadratic moments $[ii]$ $(i = 1,2,\ldots,k)$ of order 2 are equal to $\lambda_2 = 1$.

Thus the moment matrix is

$$N^{-1}[\underline{X}'\underline{X}] = \begin{bmatrix} 1 & [1] & [2] & \cdots & [k] \\ [1] & [11] & [12] & \cdots & [1k] \\ [2] & [12] & [22] & \cdots & [2k] \\ \vdots & \vdots & \vdots & & \vdots \\ [k] & [1k] & [2k] & \cdots & [kk] \end{bmatrix} = \underline{I}_{k+1} \qquad (65)$$

N^{-1}

and a first order rotatable design is one whose moment matrix is the unit matrix. Consequently such a design is obtained by writing down any k vectors mutually orthogonal to a column vector of ones, and each of which is standardized so that $(N-1)\sum_{u=1}^{N} x_{iu}^2 = 1$. We notice that this is the same conclusion (Plackett and Burman; 1946, Box; 1952) which is reached if we pursue an apparently different objective, namely if we select a design which supplies estimates $b_0, b_1, \ldots, b_k$ having smallest variance. The information distribution for such a design is

$$I(\hat{y}) = \frac{\sigma^2}{1+\rho^2} \rightarrow \sigma^{-2} \qquad \text{where} \qquad \rho^2 = \sum_{i=1}^{k} x_i^2 \qquad (66)$$

In Figure (4) below the information distribution is shown, $I(\hat{y})$ being plotted against ρ, and we see that in this example the fall-off in information as we move away from the origin follows the Cauchy distribution.

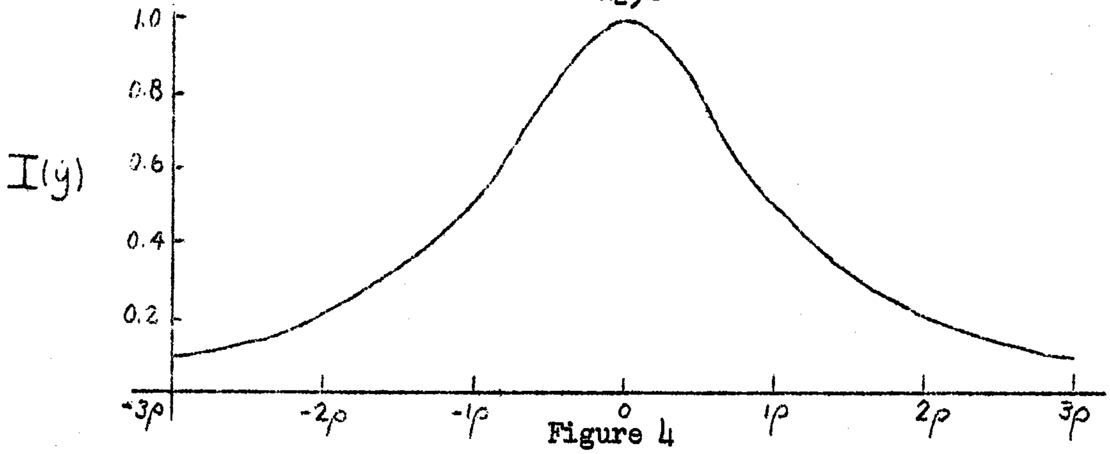


Figure 4

Information per observation at a distance ρ from the center of a 1^{st} order rotatable design.

5.2 ROTATABLE DESIGNS OF ORDER TWO

Suppose we have k variables, and fit a polynomial of degree two. For example, if k = 2 we have

$$\dot{y} = b_0 + b_1x_1 + b_2x_2 + b_{11}x_1^2 + b_{22}x_2^2 + b_{12}x_1x_2 \tag{67}$$

Then using (63) we know that all moments are zero in which any of the α_i are odd. The remaining moments are then $[ii] = \lambda_2 = 1$, $[iijj] = \lambda_4$, $[iiii] = 3\lambda_4$. Thus, for example, if k = 2

$$N^{-1}[\underline{X}'\underline{X}] = \begin{bmatrix} 1 & [1] & [2] & [11] & [22] & [12] \\ [1] & [11] & [12] & [111] & [122] & [112] \\ [2] & [12] & [22] & [112] & [222] & [122] \\ [11] & [111] & [112] & [1111] & [1122] & [1112] \\ [22] & [122] & [222] & [1122] & [2222] & [1222] \\ [12] & [112] & [122] & [1112] & [1222] & [1122] \end{bmatrix} = \begin{bmatrix} 1 & \cdot & \cdot & 1 & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & 3\lambda & \lambda & \cdot \\ 1 & \cdot & \cdot & \lambda & 3\lambda & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \lambda \end{bmatrix} \tag{68}$$

where λ is written for λ_4.

In general, for every value of k the matrix $N^{-1}[\underline{X}'\underline{X}]$ will be of the same form, in which the only mixed moments that occur are those corresponding to the variables $x_0, x_1^2, x_2^2, \ldots, x_k^2$. The measure of kurtosis for this design pattern is $\gamma_2 = 3(\lambda - 1)$. We notice in particular that if the design is to be orthogonal in the sense of § (2) as well as rotatable then using (19) $\lambda_4 = 1$, $\gamma_2 = 0$ and the moments of the design to order $2d = 4$ are the same as those as the spherical multinormal distribution.

To determine the inverse matrix $N[\underline{X}'\underline{X}]^{-1}$ we partition off a $(k + 1) \times (k + 1)$ sub matrix $\underline{U}$ of $N^{-1}[\underline{X}'\underline{X}]$ corresponding to the variables $x_0, x_1^2, x_2^2, \ldots, x_k^2$.

$$\underline{U} = \begin{bmatrix} 1 & 1 & 1 & \ldots & 1 \\ 1 & 3\lambda & \lambda & \ldots & \lambda \\ 1 & \lambda & 3\lambda & \ldots & \lambda \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ 1 & \lambda & \lambda & \ldots & 3\lambda \end{bmatrix} \tag{69}$$

for which the inverse is readily shown to be

$$U^{-1} = A \begin{bmatrix} 2\lambda^2(k+2) & -2\lambda & -2\lambda & \ldots & -2\lambda \\ -2\lambda & (k+1)\lambda-(k-1) & 1-\lambda & \ldots & 1-\lambda \\ -2\lambda & 1-\lambda & (k+1)\lambda-(k-1) & \ldots & 1-\lambda \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ -2\lambda & 1-\lambda & 1-\lambda & \ldots & (k+1)\lambda-(k-1) \end{bmatrix} \tag{70}$$

where $A = [2\lambda\{(k + 2)\lambda - k\}]^{-1}$ (71)

The remaining elements in $N^{-1}[\underline{X}'\underline{X}]$ are the diagonal elements corresponding to linear and interaction terms. The reciprocal $N[\underline{X}'\underline{X}]^{-1}$ consists of the elements $\underline{U}^{-1}$ with the reciprocals of these remaining diagonal elements. For the general second order rotatable design therefore we have

$$NV(b_0) = 2\lambda^2(k+2)A\sigma^2;\ NV(b_i) = \sigma^2;\ NV(b_{ii}) = [(k+1)\lambda - (k-1)]A\sigma^2;\ NV(b_{ij}) = \lambda^{-1}\sigma^2$$

$$NCov(b_0, b_{ii}) = -2\lambda A\sigma^2;\quad NCov(b_{ii}b_{jj}) = (1-\lambda)A\sigma^2 \tag{72}$$

and all the remaining covariances are zero. We see that for any rotatable second order design, all first and second degree effects will be un-correlated except the quadratic effects which are correlated with each other, with coefficient of correlation $\left\{\frac{2}{1-\lambda} - (k+1)\right\}^{-1}$. We see that for any value of λ the matrix $(\underline{X}'\underline{X})^{-1}$ is of a simple form and experiments carried out with such designs would be readily analysed.

If the design is rotatable and orthogonal so that $\lambda = 1$ these correlations vanish and we have

$$NV(b_0) = \tfrac{1}{2}(k+\overset{2}{\cancel{1}})\sigma^2;\quad NV(b_i) = \sigma^2;\quad NV(b_{ii}) = \tfrac{1}{2}\sigma^2;\quad NV(b_{ij}) = \sigma^2;\ NCov(b_0b_{ii}) = -\tfrac{1}{2}\sigma^2 \tag{73}$$

The condition of rotatability and orthogonality fixes the relative values for effects of different orders. In particular for designs of this sort the variances of the quadratic effects b_{ii} are 1/2 those of the two-factor interaction effects b_{ij}. They may be compared with three-level factorial designs for which the variance of the quadratic effects is twice that for the interaction. Compared with the factorial the rotatable orthogonal design thus places four times as much emphasis on the quadratic effects relative to the interaction effects.

The information distribution for any the second order rotatable design is given by

$$I(\dot{y}) = \left[A\left\{2(k+2)\lambda^2 + 2\lambda(\lambda-1)(k+2)\rho^2 + [(k+1)\lambda - (k-1)]\rho^4\right\}\right]^{-1} \Big/ \sigma^2 \tag{74}$$

In particular, for the rotatable orthogonal design this is

$$I(\dot{y}) = \left\{\frac{1}{2}\left[k + 2 + \rho^4\right]\right\}^{-1} \Big/ \sigma^2$$

In Figure 5 $I(\dot{y})$ is plotted against ρ for various values of λ. We notice that whatever value of λ is chosen the information falls off rapidly when ρ exceeds unity. If we chose $\lambda = 1$ the design will be orthogonal. For this and other higher values of λ the distribution has a large value in the center and the information will generally be slightly greater than it is for the lower values of λ even when ρ exceeds one. It is perhaps well to remember at this point, however, that we are comparing designs for which the "spread" of points, as measured by the marginal second moments $S_i^2 = N^{-1} \sum_{u=1}^{N} (X_{iu}^2 - \bar{X}_i)^2$ is constant. Such a convention is bound to favor designs with a high value of γ_2, so that although the general shape of the information distribution will be meaningful, the relative heights of the curves will be to some extent an outcome of this convention. It seems reasonable to ask for a relatively uniform distribution of information in the immediate vicinity of the design. In particular, if the information at $\rho = 1$ is to equal the information at $\rho = 0$, the following values of λ_4 will be needed

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

Table 3: Values of λ_4 Required to Make the Amount of Information at $\rho = 1$ Equal to the Amount of Information at $\rho = 0$.

6. DERIVATION OF 2nd ORDER ROTATABLE DESIGNS

The above discussion had been directed to deciding what type of design we should be seeking. It has appeared that a second order rotatable design with a value of λ which gave a fairly uniform distribution of information between ρ equals

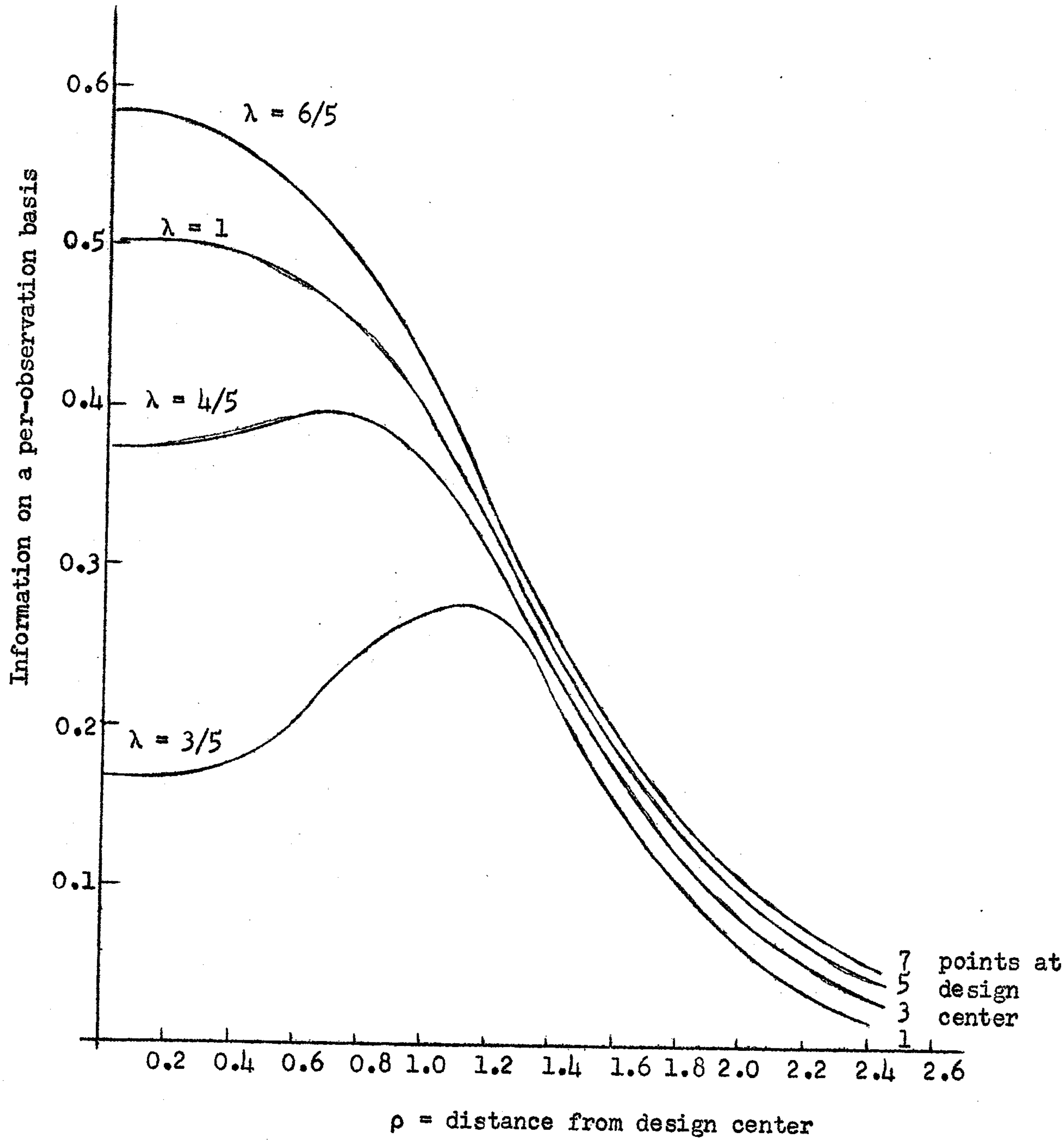


Figure 5

Information per observation at a distance ρ from the origin for second order rotatable designs with various values of λ

zero and ρ equals one would be satisfactory. We now consider how designs of this type may be obtained.

We have seen that for a spherical distribution of information the moments of the design must be the same as those of a spherical probability distribution up to order 2d. If such arrangements are obtainable, therefore, we might expect to construct them by trying, as nearly as is possible with a finite number of points, to form a spherical distribution, that is, a distribution in which the density of the points is constant on spheres. The nearest we might expect to come to this with a finite number of points would be an arrangement with the points equally spaced over the spheres. We shall need, therefore, to consider the moment properties of the regular figures in k dimensional space.

We shall find that it is often convenient to regard the designs as built up from component sets of points. In what follows such a component set shall be called an "arrangement". If the arrangement satisfies the moment conditions for rotatability up to order 2d, we shall say that it is a rotatable arrangement of order d.

It is important to remember that n points at the origin provide a rotatable arrangement of infinite order.

6.1 ARRANGEMENTS WITH ALL POINTS EQUI-DISTANT FROM THE ORIGIN

We shall find that it is possible to obtain rotatable arrangements, i.e. arrangements that satisfy the moment conditions (63), by using n points, each of which is the same distance ρ from the origin. Such arrangements by themselves cannot provide second order designs. This is seen as follows:

The sum of squares of elements in the u^{th} row of the design matrix for such arrangement is ρ^2, whence

$$n^{-1}\sum_{u=1}^{n}\sum_{i=1}^{k} x_{iu}^2 = \sum_{i=1}^{k} [ii] = \rho^2 \tag{76}$$

If therefore $[ii] = [jj]$, $(i, j, = 1,2,\ldots,k)$ then

$$[ii] = \rho^2/k \tag{77}$$

Also

$$n^{-1} \sum_{u=1}^{n} \left\{ \sum_{i=1}^{k} (x_{iu}^2) \right\}^2 = \sum_{i=1}^{k} [iiii] + \sum_{i=1}^{k} \sum_{i \neq j}^{k} [iijj] = \rho^4 \tag{78}$$

But from (69), if the arrangement is rotatable (78) must also be equal to

$$3k\lambda + k(k - 1)\lambda \tag{79}$$

Whence

$$\lambda = \rho^4/k(k + 2) \tag{80}$$

If we attempt to use such an arrangement as a second order design then putting $[ii] = 1$, $(i = 1,2,\ldots,k)$ we have $\rho^2 = k$, whence

$$\lambda = k/k + 2 \tag{81}$$

$$\gamma_2 = -6/(k + 2) \tag{82}$$

Using (71) for such a value of λ, A is infinite and the quadratic effects are not estimable.

By combining two or more such arrangements, however, we shall see that designs may be obtained for which the value of λ is not pathological.

6.2 COMBINATION OF ARRANGEMENTS

Suppose we combine s, k-dimensional arrangements (not necessarily rotatable arrangements of order two) to form a rotatable design of order two. Suppose the w^{th}

such arrangement contains n_w points all at a distance ρ_w (and $\sum_{w=1}^{S} n_w = N$), and that the marginal second moments are all equal, (and hence are given by $[ii]_w = \rho_w^2/k$). Suppose finally that for the w^{th} arrangement the measure of kurtosis of the variable x_i is γ_{2wi}, so that $[iiii]_w = \dfrac{(3+\gamma_{2wi})\rho_w^4}{k^2}$

Then for the entire design

$$[ii] = (kN)^{-1} \sum_{w=1}^{S} n_w \rho_w^2 \tag{83}$$

$$[iiii] = (k^2N)^{-1} \sum_{w=1}^{S} n_w \rho_w^4 \, (3 + \gamma_{2wi}) \tag{84}$$

Putting $[ii] = 1$ we have for the measure of kurtosis γ_{2i} for the variable x_i in the complete design

$$3 + \gamma_{2i} = \frac{N \sum_{w=1}^{S} n_w \rho_w^4 \, (3 + \gamma_{2wi})}{\left(\sum_{w=1}^{S} n_w \rho_w^2\right)^2} \tag{85}$$

Whence, if by combining such arrangements we can attain a second order rotatable design, this expression is equal to 3λ, that is

$$\lambda = \frac{1}{3}\gamma_{2i} + 1 \tag{86}$$

We note that for n_1 points in the center the term $\rho_1^4(3 + \gamma_{21i})$ in (85) equals $k^2[iiii]_1$ which is zero.

7. TWO DIMENSIONAL DESIGNS

Consider n equally spaced points on a circle of radius ρ in the complex plane, and suppose the first point makes an angle φ with the real axis, then if M_p is the p^{th} moment of the projections of the n points on the real axis

$$nM_p(\varphi) = \rho^p \sum_{u=0}^{n-1} \left\{ \cos(\varphi + u\theta) \right\}^p \tag{87}$$

where θ is the angle between radii from the origin to successive points,

$$nMp(\varphi) = (\tfrac{1}{2}\rho)^p \sum_{u=0}^{n-1} (a\omega^u + a^{-1}\omega^{-u})^p \tag{88}$$

where $$e^{i2\pi/n} = e^{i\theta} = \omega, \quad e^{i\varphi} = a, \quad \omega^n = 1 \tag{89}$$

that is

$(\binom{p}{t})$

$$nMp(\varphi) = (\tfrac{1}{2}\rho)^p \sum_{u=0}^{n-1} \sum_{t=0}^{p} \binom{p}{t} (a\omega^u)^{p-t} (a\omega^u)^{-t} \tag{90}$$

$$= (\tfrac{1}{2}\rho)^p \sum_{u=0}^{n-1} \sum_{t=0}^{p} \binom{p}{t} a^{p-2t}\, \omega^{(p-2t)u} \tag{91}$$

If $\varphi = 0$, $a = 1$ and substituting this value in (91) and substracting the result from (91) we obtain an expression for the change in the p^{th} moment on rotating through an angle φ,

$$n \quad M_p(\varphi) - M_p(0) = (\tfrac{1}{2}\rho)^p \sum_{u=0}^{n-1} \sum_{t=0}^{p} \binom{p}{t} \omega^{(p-2t)u} \quad (a^{p-2t} - 1) \tag{92}$$

$$= (\tfrac{1}{2}\rho)^p \sum_{t=0}^{p} \binom{p}{t} (a^{p-2t} - 1) \sum_{u=0}^{n-1} \omega^{(p-2t)u} \tag{93}$$

Now $\sum_{u=0}^{n-1} \omega^{(p-2t)u}$ = n whenever p - 2t is 0 or mn, where m is any positive or negative integer

$$= \frac{\omega^{n(p-2t)} - 1}{\omega^{p-2t} - 1} = 0 \text{ otherwise .} \tag{94}$$

We see therefore, since for t = 0, 1, 2, ..., p, we have $-p \leq p - 2t \leq p$, then if $p < n$ all moments on the real axis are invariant under rotation. For if $p - 2t = 0$, so that (94) yields a non-zero product, $(a^{p-2t} - 1)$ in (93) is zero. We notice however, that for $p > n$ the moments on the real axis will not in general be invariant under rotation.

Thus for a set of equally spaced points on a circle the marginal moments of the projections on any axis through the center remain constant. It follows that the moments and the mixed moments of the two-dimensional arrangements up to order $n - 1$ are constant for any set of orthogonal axes through the origin and consequently they are of the form (68). Hence n equally spaced points on a circle provide a rotatable arrangement of order $(n - 1)/2$. In particular 5 or more points arranged in a regular polygon gives a rotatable arrangement of order 2.

Since the points are all equidistant from the origin, however, we know from § 6.1 that we could not use such an arrangement as a second order design. For, with these points alone, the quadratic effects are not estimable. This is readily confirmed for the particular case $k = 2$ for if p is even, the only non-zero element in (91) is $(\frac{1}{2}\rho)^p \binom{p}{p/2} n$ thus

$$M_p = (\tfrac{1}{2}\rho)^p \frac{p!}{(\frac{1}{2}p)!\,(\frac{1}{2}p)!} \tag{95}$$

which using equation (43), is the p^{th} marginal moment for the spherical distribution for which

$$\lambda_p = \frac{1}{(\frac{1}{2}p)!} \cdot \left(\frac{\rho^2}{2}\right)^{\frac{p}{2}} \tag{96}$$

If $[11] = [22] = 1$, $\rho = \sqrt{2}$ and $\lambda_p = \dfrac{1}{(\frac{1}{2}p)!}$ and in particular $\lambda_4 = 1/2$, $\gamma_2 = -1.5$, a pathological value. For more than one circle of points however substituting $\gamma_{2wi} = -1.5$ in (85) we have

$$\left(\sum_{w=1}^{S} n_w \rho_w^2\right)^2 \lambda = \frac{1}{2} N \sum_{w=1}^{S} n_w \rho_w^4 \tag{97}$$

a formula which clearly applies also when n_1 of the points are at the center (when ρ_1 equals zero). Substituting any desired value of λ in (91) produces an equation any solution of which with $n_1 > 0$ and $n_w \geqslant 5$, $(w = 2,3,\ldots,s)$ produces the desired second order rotatable design. It is clear that an infinity of solution of (97) will exist. Those which involve the fewest number of points will have one circle of n_2 = five points with n_1 points at the center.

The value of λ for any value of n_1 is then

$\frac{n_1}{n_2})$

$$\lambda = \frac{1}{2}(n_1 + n_2)\,\frac{n_2\rho_w^4}{n_2^2\rho_w^4} = \frac{1}{2}\,\frac{n_1+n_2}{n_2} = \frac{1}{2}\left(1 + \frac{n_2}{n_1}\right) \tag{98}$$

Thus putting $n_2 = 5$ we have, in particular,

Number of points in center of pentagon (n_1)	0	1	3	5
Value of λ	1/2	3/5	4/5	1.0

Table 4: Values of λ for Points in Center of Pentagon.

It is seen that a very satisfactory design, in a sense discussed in § 5, is obtained with $n_1 = 3$. This arrangement with five points at the vertices of a pentagon and with three points at the center provides a design (see Table 3) giving about the same amount of information at $\rho = 0$ as at $\rho = 1$. For orthogonality and rotatability we require $\lambda = 1$ which gives 5 points in the center.

Orthogonal arrangements which however involve more than ten points may be obtained using two concentric circles containing $n_1 \geqslant 5$, $n_2 \geqslant 5$, at distances ρ_1 and ρ_2 from the center which satisfy (97)

n_1	5	5	5	5	6	6	6	7	7	8
n_2	5	6	7	8	6	7	8	7	8	8
ρ_1	2.000	2.047	2.089	2.128	2.000	2.040	2.076	2.000	2.034	2.000
ρ_2	0	0.417	0.557	0.647	0	0.385	0.518	0	0.359	0

Table 5: Designs in Two Concentric Circles

8. SECOND ORDER DESIGNS IN MORE THAN TWO DIMENSIONS

There exist only a limited number of regular figures in k dimensions. In particular, in three dimensions there are only the tetrahedron, n = 4; octahedron, n = 6; cube, n = 8; icosahedron, n = 12; and the dodecahedron with n = 20 points. The tetrahedron, octahedron and cube are not capable of forming alone a basis for a second order design, but there remains the possibility that two or more such arrangements suitably combined, with suitable values of ρ, might provide second order arrangements. We should, therefore, consider the moment matrices for regular figures submitted to a general rotation defined by the k x k orthogonal matrix $\underline{H}$. Given any N x k design matrix $\underline{D}$, the points making up the design may be generally rotated by post-multiplying $\underline{D}$ by $\underline{H}$. Similarly the moment matrix $N^{-1}\,\underline{X}'\underline{X}$ associated with a polynomial model of order d is transformed by rotation to a new moment matrix by pre and post-multiplying $N^{-1}\,\underline{X}'\underline{X}$ by an orthogonal matrix derived from $\underline{H}$. For a second degree k dimensional model the moment matrix after the rotation of the design is

$$N^{-1}\begin{bmatrix} 1 & & \\ & \underline{H} & \\ & & \underline{H}^{[2]} \end{bmatrix}' \underline{X}'\underline{X} \begin{bmatrix} 1 & & \\ & \underline{H} & \\ & & \underline{H}^{[2]} \end{bmatrix} \qquad (99)$$

where $\underline{H}^{[2]}$ is the second Schläflian matrix; i.e., if

$$\underline{H} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \tag{100}$$

The second Schläflian $H^{[2]}$ may be written in abbreviated form as

$$\left[\begin{array}{c:c} \underline{\alpha} & \underline{\beta} \\ \hdashline \underline{\gamma} & \underline{\delta} \end{array}\right] \tag{101}$$

where the partition is made after the k^{th} row and column and where

$$\underline{\alpha} = \begin{bmatrix} a_{11}^2 & a_{21}^2 & a_{31}^2 \\ a_{12}^2 & a_{22}^2 & a_{32}^2 \\ a_{13}^2 & a_{23}^2 & a_{33}^2 \end{bmatrix}$$

$$\underline{\beta} = \begin{bmatrix} \sqrt{2}a_{11}a_{21} & \sqrt{2}a_{11}a_{31} & \sqrt{2}a_{21}a_{31} \\ \sqrt{2}a_{12}a_{22} & \sqrt{2}a_{12}a_{32} & \sqrt{2}a_{22}a_{32} \\ \sqrt{2}a_{13}a_{23} & \sqrt{2}a_{13}a_{33} & \sqrt{2}a_{23}a_{33} \end{bmatrix}$$

$$\underline{\gamma} = \begin{bmatrix} \sqrt{2}a_{11}a_{12} & \sqrt{2}a_{21}a_{22} & \sqrt{2}a_{31}a_{32} \\ \sqrt{2}a_{11}a_{13} & \sqrt{2}a_{21}a_{23} & \sqrt{2}a_{31}a_{33} \\ \sqrt{2}a_{12}a_{13} & \sqrt{2}a_{22}a_{23} & \sqrt{2}a_{32}a_{33} \end{bmatrix} \tag{102}$$

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

Since $\underline{H}$ is orthogonal, it can be easily shown that

$$\underline{\alpha}'\underline{\beta} = -\underline{\gamma}'\underline{\delta}, \quad \underline{\gamma}'\underline{\gamma} = \underline{I} - \underline{\alpha}'\underline{\alpha}, \quad \underline{\beta}'\underline{\beta} = \underline{I} - \underline{\delta}'\underline{\delta}$$

To correspond to our definition of derived power vectors and Schläflians we write the model in the form in which the product terms $x_i x_j$ are written with a coefficient $\sqrt{2}$, for example for $k = 3$

$$\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \frac{\beta_{12}}{\sqrt{2}} (\sqrt{2} x_1 x_2) + \frac{\beta_{13}}{\sqrt{2}} (\sqrt{2} x_1 x_3) + \frac{\beta_{23}}{\sqrt{2}} (\sqrt{2} x_2 x_3)$$

We may now investigate the moment matrices of the regular figures under any rotation. It has been shown previously, § 5, that the moment matrix $N^{-1}\underline{X}'\underline{X}$ for any rotatable design of second degree in k dimensions must be, (with the present definition of the interaction variables) of the form

$$N^{-1}[\underline{X}'\underline{X}] = \begin{bmatrix}
1 & & & & & 1 & 1 \cdots & 1 & & & & \\
 & 1 & & & & & & & & & & \\
 & & 1 & & & & & & & & & \\
 & & & \ddots & & & & & & & & \\
 & & & & 1 & & & & & & & \\
 & & & & & 3\lambda & \lambda \cdots & \lambda & & & & \\
 & & & & & & 3\lambda \cdots & \lambda & & & & \\
 & & & & & & \ddots & 3\lambda & & & & \\
 & \text{Symmetric} & & & & & & & 2\lambda & & & \\
 & & & & & & & & & 2\lambda & & \\
 & & & & & & & & & & \ddots & \\
 & & & & & & & & & & & 2\lambda
\end{bmatrix} \qquad (103)$$

Substituting $\underline{X}'\underline{X}$ for the tetrahedron in (99) and solving for the moment matrix of the generally rotated matrix of the tetrahedron, all of whose points are on a sphere of radius $\sqrt{3}$, we have

$$\frac{1}{4}\underline{X}'\underline{X} = \left[\begin{array}{c|c|c|c} 1 & 0 & 1\,1\,1 & 0 \\ \hline 0 & \underline{I}_3 & \sqrt{2}\,\underline{H}'\underline{J}\,\underline{\gamma} & \sqrt{2}\,\underline{H}'\underline{J}\underline{\delta} \\ \hline \begin{matrix}1\\1\\1\end{matrix} & \underline{\gamma}'\underline{J}'\underline{H}\sqrt{2} & \underline{1}\underline{1}'+2\underline{\gamma}'\underline{\gamma} & 2\underline{\gamma}'\underline{\delta} \\ \hline 0 & \underline{\delta}'\underline{J}'\underline{H}\sqrt{2} & 2\underline{\delta}'\underline{\gamma} & 2\underline{\delta}'\underline{\delta} \end{array}\right] \tag{104}$$

where $\underline{J}$ is a k x k matrix such that $\underline{J}\underline{J}' = \underline{I}$, thus for k = 3 we have

$$\underline{J} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \tag{105}$$

and the vector $\underline{1}$ is a column vector all of whose elements are unity so that the matrix $\underline{1}\underline{1}'$ is a k x k matrix all of whose elements are ones, that is when k = 3

$$\underline{1}\underline{1}' = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \tag{106}$$

We see that the moment matrix for the generally rotated tetrahedron satisfies the moment requirements up to order two, but not up to order four required for a rotatable arrangement of second order.

The moment matrices for the generally rotated octahedron and cube with $\rho = \sqrt{3}$ are

$$\frac{1}{6}\left[\underline{X}'\underline{X}\right] = \left[\begin{array}{c|c|c|c} 1 & 0 & 1\,1\,1 & 0 \\ \hline 0 & \underline{I}_3 & 0 & 0 \\ \hline \begin{matrix}1\\1\\1\end{matrix} & 0 & 3\underline{\alpha}'\underline{\alpha} & 3\underline{\alpha}'\underline{\beta} \\ \hline 0 & 0 & 3\underline{\beta}'\underline{\alpha} & 3\underline{\beta}'\underline{\beta} \end{array}\right] \qquad \frac{1}{8}\left[\underline{X}'\underline{X}\right] = \left[\begin{array}{c|c|c|c} 1 & 0 & 1\,1\,1 & 0 \\ \hline 0 & \underline{I}_3 & 0 & 0 \\ \hline \begin{matrix}1\\1\\1\end{matrix} & 0 & \underline{1}\underline{1}' + 2\underline{\gamma}'\underline{\gamma} & 2\underline{\gamma}'\underline{\delta} \\ \hline 0 & 0 & 2\underline{\delta}'\underline{\gamma} & 2\underline{\delta}'\underline{\delta} \end{array}\right] \qquad (107)$$

OCTAHEDRON CUBE

These matrices both satisfy the moment requirements for rotatability up to order two, but not up to order four required for a second order rotatable arrangement.

The moment matrices for the generally rotated icosahedron and dodecahedron with $\rho = \sqrt{3}$ are of the form

$$\frac{1}{N}\,\underline{X}'\underline{X} = \left[\begin{array}{c|c|c|c} 1 & 0 & 1\;1\;1 & 0 \\ \hline 0 & \underline{I}_3 & 0 & 0 \\ \hline \begin{matrix}1\\1\\1\end{matrix} & 0 & \frac{6}{5}\underline{I}_3 + \frac{3}{5}\,\underline{1}\underline{1}' & 0 \\ \hline 0 & 0 & 0 & \frac{6}{5}\,\underline{I}_3 \end{array}\right]$$

where N = 12 for the icosahedron

N = 20 for the dodecahedron

The moment matrices for the generally rotated icosahedron and dodecahedron do oblige all the moment requirements up to order four necessary for a second order rotatable arrangement. However, as outlined in § 6.1 any arrangement of points, all of which are the same distance from the origin, cannot provide a second order design since the mean and quadratic effects are not estimable. In fact we note that $\lambda = 3/5 = k/(k + 2)$ agreeing with (72).

However, as indicated in § 6.1, different arrangements of points may be combined to give workable rotatable designs. The problem now is to change the γ_2 (i.e., the λ) of the designs without affecting the relative magnitudes of the moments of the same order. This is most economically accomplished by adding n_1, new points at the center of the design. Adding n_1 new points at the center yields for the complete arrangement

$$3\lambda = (n_1 + n_2)\frac{\sum x_i^4(3+\gamma_{22i})}{(\sum x_i^2)^2} \text{ or } \lambda = \left(1+\frac{n_1}{n_2}\right)\frac{3}{5}$$

In particular, to guarantee an approximately uniform distribution of information throughout the interior of the design, we note from Table 3 that we require $\lambda = 0.84$, which is most nearly attained with $n_1 = 5$ points for the icosahedron, and $n_1 = 8$ points for the dodecahedron, thus giving designs requiring a total of 17 and 28 points respectively. For an orthogonal rotatable design $\lambda = 1$ which requires $n_1 = 8$ for the icosahedron and $n_1 = 40/3$ (or 13 to the nearest integer) for the dodecahedron.

It can be shown (H.S.M. Coxeter, Regular Polytopes, Methuen and Co., Ltd. 1948) that the twenty points forming the dodecahedron may be divided into five sets of four points, each of these sets being a tetrahedron, that is, five tetrahedra may be inscribed in a dodecahedron. As indicated in § 6.1, given that for each of the arrangements all the points are equidistant from the origin, rotatable designs are possible by combining such arrangements. Thus if we imagine five tetrahedra defined by suitable rotations $\underline{H}_1, \underline{H}_2, \ldots, \underline{H}_5$, the sum of the five resultant matrices (104) will give the moment matrix of a rotatable arrangement.

A further example of a combination of sets of points not themselves second order rotatable arrangements which together form such a configuration is provided by the octahedron and the cube. Taking advantage of the fact that $\underline{\alpha}'\underline{\beta} = -\underline{\gamma}'\underline{\delta}$ we may add the two moment matrices of the cube and octahedron together, (107), so that the quadratic by interaction elements in the resultant matrix become zero, making sure to guarantee that $18\rho_1^4 \underline{\alpha}'\underline{\beta} = 16\rho_2^4 \underline{\gamma}'\underline{\delta}$ where ρ_1 is the radius of the octahedron and ρ_2 is the radius of the cube. Thus, if the points of the cube are on a sphere of radius $\sqrt{3}$, the points of the octahedron must lie on a sphere of radius $2^{3/4}$. The resultant moment matrix is

$$\frac{1}{14}\,\underline{X}'\underline{X} = \left[\begin{array}{c|c|c|c} 1 & & 1 \quad 1 \quad 1 & \\ \hline & I_3 & & \\ \hline \begin{matrix}1\\1\\1\end{matrix} & & \frac{14}{2(3+2\sqrt{2})} I_3 + \frac{7}{2(3+2\sqrt{2})} 11' & \\ \hline & & & \frac{7}{2(3+2\sqrt{2})} I_3 \end{array}\right]$$

and $\lambda = \dfrac{7}{2(3+2\sqrt{2})} = 0.60050$

This value of λ is very close to the pathological value of $\lambda = k/(k+2) = 0.6$, thus although the quadratic effects are theoretically estimable, their variances would be extremely large. Proceeding as before, a design with an approximately uniform information distribution can be obtained by adding $n_1 = 5.6$ (i.e., 6 to the nearest integer) points at the origin. Similarly, a nearly orthogonal rotatable design is obtained using $\lambda = 1$, which gives $n_1 = 9.3$ (i.e., 9 points) to the origin.

The combining of the octahedron and the cube to form a second order rotatable design is of particular importance since figures analagous to the octahedron and the cube are available in k dimensions.

In four dimensions the regular figures comprise that formed from five points, the analogue of the tetrahedron; the next in the series is that formed from 8 points, the four dimensional analogue of the octahedron; that formed from 16 points, the four dimensional analogue of the cube; and a further figure formed from 24 points which, as we shall see later, can be formed by combining the "cube" and "octahedron".

Other regular figures occur but these have at least 120 points and are not of value for the present purpose. Proceeding as before, the moment matrix for the generally rotated 8 point figure is

$$\frac{1}{8}\,\underline{X}'\underline{X} = \left[\begin{array}{c|c|c|c} 1 & & 1\;1\;1\;1 & \\ \hline & \underline{I}_4 & & \\ \hline \begin{matrix}1\\1\\1\\1\end{matrix} & & 4\,\underline{\alpha}'\underline{\alpha} & 4\underline{\alpha}'\underline{\beta} \\ \hline & & 4\,\underline{\beta}'\underline{\alpha} & 4\underline{\beta}'\underline{\beta} \end{array}\right] \tag{111}$$

The moment matrix for the 16 point figure is

$$\frac{1}{16}\,\underline{X}'\underline{X} = \left[\begin{array}{c|c|c|c} 1 & & 1\;1\;1\;1 & \\ \hline & \underline{I}_4 & & \\ \hline \begin{matrix}1\\1\\1\\1\end{matrix} & & 2\underline{\gamma}'\underline{\gamma} + \underline{1}\underline{1}' & 2\;\underline{\gamma}'\underline{\delta} \\ \hline & & 2\underline{\delta}'\underline{\gamma} & 2\;\underline{\delta}'\underline{\delta} \end{array}\right] \tag{112}$$

while that for the 24 point figure is

$$\frac{1}{24}\,\underline{X}'\underline{X} = \left[\begin{array}{c|c|c|c} 1 & & 1\;1\;1\;1 & \\ \hline & \underline{I}_4 & & \\ \hline \begin{matrix}1\\1\\1\\1\end{matrix} & & \frac{4}{3}\,\underline{I}_4 + \frac{2}{3}\,\underline{1}\underline{1}' & \\ \hline & & & \frac{4}{3}\,\underline{I}_4 \end{array}\right] \tag{113}$$

This latter configuration is seen to form a rotatable arrangement of second order with $\lambda = 2/3$ from which may be formed a rotatable design. Proceeding as before, we find by adding points to the center a suitable value of λ may be obtained. In particular, we find to attain the value of $\lambda = 0.87$, (Table 3) required for a reasonably uniform distribution of information within the design requires $n_1 = 7.32$, i.e, 7 points. The number of points required for $\lambda = 1$, necessary for orthogonality, is $n_1 = 12$.

The 8 point regular figure and the 16 point regular figure are clearly not rotatable arrangements of order two, but following the device recorded in the last section, may be combined to form such an arrangement. Proceeding as before we find that the values of the radii of the two figures must be equal, and that the arrangement is the same as that obtained from the 24 point regular figure.

8.1. DESIGNS IN MORE THAN FOUR DIMENSIONS

In more than four dimensions only three regular figures exist, these are the regular simplex involving k + 1 points, which is the analogue of the tetrahedron; the cross polytope which is the analogue of the octahedron with 2k points; and the measure polytope, the hypercube, with 2^k points. Configurations corresponding to the icosahedron and the dodecahedron are not now available. We may, however, always form a rotatable arrangement by combining the cross-polytope and the measure polytope. It can further be shown that if the points of a k-dimensional measure polytope are on a hyper-sphere of radius $\sqrt{k}$, the points of the k-dimensional cross polytope necessary to form a rotatable second order design will be on hyper-sphere of radius $2^{k/4}$. The table below shows the number of points required at the center of the design to attain a rotatable arrangement for values of λ required to give approximately uniform information, and for orthogonality.

	k	4	5	6	7	8
	n_2	24	42	76	142	273
n_1	added points at center for approximately uniform information	7	10	16	24	43
n_1	added points at center for orthogonality	12	17	24	35	48

Table 6: Uniform Information and Orthogonal Designs for $k \geq 4$.

The number of points required in such designs, although far fewer than the three level factorial arrangement, nevertheless rapidly becomes much greater than the number of constants to be estimated. It is often possible however to produce the same moment matrix up to order 2d as is given by the hypercube (the 2^k design) using a fraction of the points of the hypercube. Such arrangements are the fractional two-level factorials which may be combined with the points of the cross-polytope to give second order arrangements. In particular, for k = 5, 6 and 7, a 1/2 replicate of the 2^k design may be used, and for k = 8, a 1/4 replicate may be used. These arrangements with appropriate values of λ are given in Table 7. Whenever a 1/2 replicate of the hypercube is used, if all the points on the hypercube lie on a sphere of $(\text{radius})^2 = k$, then all the points of the cross-polytope necessary for a second order rotatable design lie on a sphere of $(\text{radius})^2 = 2^{\frac{k-1}{2}}$. Whenever a 1/4 replicate of the hypercube is used then the $(\text{radius})^2$ of the required cross polytope is $= 2^{\frac{k-2}{2}}$, and in general a $(\frac{1}{2})^p$ replicate of a hypercube in k dimensions requires a cross polytope in k dimensions with a $(\text{radius})^2 = 2^{\frac{k-p}{2}}$.

These arrangements, with appropriate values of n_1 required for approximately uniform information distributions within the design, and for orthogonality are given in the table below

		1/2 replicate				1/4 replicate
	k	5	6	7	8	8
	n_2	26	44	78	144	80
n_1	added points at the center for approximately uniform information	6	8	12	20	4
n_1	added points at the center for orthogonality	10	17	22	33	20
	$\frac{(\text{radius})^2 \text{ of Cross Polytope}}{(\text{radius})^2 \text{ of Hypercube}}$	$\frac{4}{5}$	$\frac{2\sqrt{2}}{3}$	8/7	$\sqrt{2}$	1

Table 7: Designs Using Fractional Factorials for $k \geq 5$.

9. CONFOUNDING

Situations frequently occur in practice where it is desirable to perform experiments in "blocks". This situation arises for example where an insufficient quantity of uniform material is available for use in all the experimental combinations, but smaller amounts of more uniform material are at hand. If it can be assumed that the effect of a change from one batch of material to another is to add a constant amount to the response at all levels of the variables, then by a suitable arrangement of the design it is possible to fit the response surface free of the disturbing influence of the quantity of the raw material. For m blocks, the mathematical model may be written

$$\eta = p(x_1,x_2,\ldots,x_k) + \sum_{i=1}^{m-1} \delta_i z_i \tag{114}$$

where the δ_i is the increase in the response in the i^{th} block, the value δ_m being determined by the remaining (m - 1) block constants so that $\sum_{i=1}^{m} \delta_i = 0$. The $z_i (i = 1,2,\ldots,n-1)$ constitute an N x 1 column vector containing unit elements for those points in the i^{th} block and zeros elsewhere.

If

It it is possible to obtain an arrangement such that the z's are orthogonal with the independent variables in the polynomial equation then the effects of the blocks may be eliminated without reducing the accuracy with which the constants of the surface are determined. When this is not possible it will be our object to obtain arrangements in which the block vectors have smallest possible inner products with the vectors of the independent variables. An example in which orthogonal blocking is possible is the three dimensional design formed from a dodecahedron. As has been already pointed out, the dodecahedron contains five tetrahedra which may be used as a basis for the arrangement. For example, if we employ a dodecahedron with 10 points in the center we may carry out the experiment in 5 blocks of 6 points, each block containing 4 points of a tetrahedron plus two points from the center. The analysis of variance for the design would appear as follows:

	df
Total	30
Due to Blocks	4
Constants	10
Lack of Fit	11
Error	5

For the icosahedron no orthogonal blocking arrangement has been found. However, for this design with 6 points in the center, one useful blocking scheme is obtained by splitting the icosahedron into its three component rectangles and using these together with pairs of points in the center to form the blocks. The linear and interaction effects are orthogonal to the block effects, but the quadratic effects are not orthogonal. The variances of the quadratic effects when blocking is used is $0.074\sigma^2$ compared with $0.033\sigma^2$ without blocking. The efficiency of these quadratic estimates is thus reduced by 56.3%.

10. ALIASES

If a function can be described using a third order polynomial model, but only a second order polynomial model has been fitted, then the estimates of the coefficients in the fitted second degree model will be biassed by the unestimated third order effects. It is of real interest therefore to investigate second order rotatable designs from the point of view of biasses contributed by third order effects.

Let $\underline{X}_1$ be the $N \times L_1$ matrix of the L_1 original independent variables, and let $\underline{X}_2$ be an $N \times L_2$ matrix of the L_2 independent variables not admitted to the original model but suspected of being required if the unknown response surface is to be properly estimated. Thus, in estimating an unknown response surface with a second order polynomial model the L_1 independent variables would be the mean, linear and second order (both quadratic and two factor interaction) effects. The L_2 independent variables would be the third order effects. It is originally assumed that the proper model is

$$\underline{\eta} = \underline{X}_1\underline{\beta}_1 \tag{115}$$

and the least squares estimates of the coefficients are then

$$\underline{B}_1 = [\underline{X}_1'\underline{X}_1]^{-1}\,\underline{X}_1'\underline{Y} \tag{116}$$

If however the correct model is

$$\underline{\eta} = \underline{X}_1\underline{\beta}_1 + \underline{X}_2\underline{\beta}_2 \tag{117}$$

then the estimates of the coefficients $\underline{B}_1$ will be biassed since

$$E(\underline{B}_1) = [\underline{X}_1'\underline{X}_1]^{-1}\,\underline{X}_1'\underline{\eta} = [\underline{X}_1'\underline{X}_1]^{-1}\underline{X}_1'\underline{X}_1\underline{\beta}_1 + [\underline{X}_1'\underline{X}_1]\underline{X}_1'\underline{X}_2\underline{\beta}_2 \tag{118}$$

thus

$$\underline{B}_1 \text{ estimates } \underline{\beta}_1 + [\underline{X}_1'\underline{X}_1]^{-1}\underline{X}_1'\underline{X}_2\underline{\beta}_2$$

$$\text{i.e. } \mathcal{E}(\underline{B}_1) = \underline{\beta}_1 + \underline{A\beta}_2 \tag{119}$$

where

$$\underline{A} = [\underline{X}_1'\underline{X}_1]^{-1}\ \underline{X}_1'\underline{X}_1 \rightarrow 2 \tag{120}$$

is called the "alias" matrix. Thus $E(b_i) = \beta_i + \sum_{j=1}^{L_2} a_{ij}\beta_j$ where b_i is any one of the original L_1 coefficients and a_{ij} is the element in the i^{th} row and j^{th} column of $\underline{A}$. Thus only those coefficients in $\underline{\beta}_1$ biassed by the added independent variables X_2 are those with non-zero elements in $\underline{A}$. Thus only those coefficients in $\underline{\beta}_1$ biassed by the added independent variables $\underline{X}_2$ are those with non-zero elements in $\underline{A}$.

<u>The Alias Matrix for Rotatable Design $k = 3$.</u>

We observe that the alias matrix can be written in the form

$$\underline{A} = N[\underline{X}_1'\underline{X}_1]^{-1}\ N^{-1}[\underline{X}_1'\underline{X}_2] \tag{121}$$

For any second order rotatable design it has been shown that $N[\underline{X}_1'\underline{X}_1]^{-1}$ is the inverse of the moment matrix of the design. In addition $N^{-1}[X_1'X_2]$ is simply a matrix of moments, and since we are concerned with rotatable designs all moments up to order four in this matrix are invarient order rotation. Thus for $k = 3$, $N^{-1}[\underline{X}_1'\underline{X}_2]$ is of the general form

$$
\begin{array}{c|cccccccccc|}
 & 111 & 222 & 333 & 122 & 133 & 112 & 233 & 113 & 223 & 123 \\
\hline
0 & & 0 & & & & 0 & & & & 0 \\
1 & 3\lambda & & & \lambda & \lambda & & & & & \cdot \\
2 & & 3\lambda & & & & \lambda & \lambda & & & \cdot \\
3 & & & 3\lambda & & & & & \lambda & \lambda & \cdot \\
11 & [11111] & [11222] & [11333] & [11122] & [11133] & [11112] & [11233] & [11113] & [11223] & [11123] \\
22 & [11122] & [22222] & [22333] & [12222] & [12233] & [11222] & [22233] & [11223] & [22223] & [12223] \\
33 & [11133] & [22233] & [33333] & [12233] & [13333] & [11233] & [23333] & [11333] & [22333] & [12333] \\
12 & [11112] & [12222] & [12333] & [11222] & [11233] & [11122] & [12233] & [11123] & [12223] & [11223] \\
13 & [11113] & [12223] & [13333] & [11223] & [11333] & [11123] & [12333] & [11133] & [12233] & [11233] \\
23 & [11123] & [22223] & [23333] & [12223] & [12333] & [11223] & [22333] & [11233] & [22233] & [12233]
\end{array}
\qquad (122)
$$

Now, provided the design is such that all 5^{th} order moments are zero, then everything in $N^{-1}[X_1'X_2]$ is zero except for the terms in the rows corresponding to the linear effects, and these are the terms that are constant in every orientation.

For any two dimensional rotatable arrangement we have seen § 7 that all moments of order $p < n$, where n is the number of equally spaced points on a circle, are invariant under rotation, and that for $p \geq n$ the moments are not in general invariant to rotation. Thus provided there are at least six points on every circle of non-zero radius, all the fifth order moments are zero. For the icosahedron, dodecahedron and the cube plus octahedron (in all dimensions) all the fifth order moments are zero.

We note now that $N[X_1'X_2]$ is of the form

$$
N[X_1'X_1]^{-1} = \left[\begin{array}{c|c|c|c}
* & 0 & * & 0 \\
\hline
0 & I_k & 0 & 0 \\
* & 0 & * & 0 \\
\hline
0 & 0 & 0 & \frac{1}{\lambda} I_k
\end{array}\right] \qquad (123)
$$

(The sub-matrices indicated by * can be derived using equation (70))

Thus, in forming the alias matrix the elements in the rows corresponding to the linear effects are multiplied only by $\underline{I}$, so that for all these designs, under all rotation, $\underline{A}$ is of the form

$$\underline{A} = \left[\begin{array}{ccc:cccccc:c}
 & 0 & & & & 0 & & & & 0 \\
\hdashline
3\lambda & & & \lambda & \lambda & & & & & \\
 & 3\lambda & & & & \lambda & \lambda & & & 0 \\
 & & 3\lambda & & & & & \lambda & \lambda & \\
\hdashline
 & 0 & & & & 0 & & & & 0 \\
\hdashline
 & 0 & & & & 0 & & & & 0
\end{array}\right] \qquad (124)$$

Thus $$\mathcal{E}(b_i) = \beta_i + \lambda(3\beta_{iii} + \sum_{i \neq j}^{k} \beta_{ijj}) \qquad (125)$$

If a fractional replicate of a cube is used with a cross polytope, the alias will be like those above, but in addition aliases of the two factor interactions with three factor interactions will also occur. For example, if $k = 5$ and we use the comfounding arrangement $I = 1{\cdot}2{\cdot}3{\cdot}4{\cdot}5$ to form a half replicate of the cube then $N^{-1}[X_1'X_2]$ for the design in its ordinary position is

$$N^{-1}[X_1'X_2] =$$

$$\begin{array}{c}
 \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 11 \\ 22 \\ \vdots \\ 55 \\ 12 \\ 13 \\ \vdots \\ 45
\end{array}
\begin{array}{c}
\begin{array}{cccccccccccccccccc}
111 & 222 & 333 & 444 & 555 & 122 & 133 & 144 & 155 & 112 & 233 & 244 & 255 & \ldots & 345 & 245 & 125 & 123 \; 125 \text{ etc}
\end{array} \\
\left[\begin{array}{ccccc:cccccccccc:cccc}
 & & 0 & & & & & & & 0 & & & & & & & & 0 & \\
\hdashline
3\lambda & & & & & \lambda & \lambda & \lambda & \lambda & & & & & & & & & & \\
 & 3\lambda & & & & & & & & \lambda & \lambda & \lambda & \lambda & & & & & & \\
 & & 3\lambda & & & & & & & & & & & \lambda & \lambda \text{ etc} & & & 0 & \\
 & & & 3\lambda & & & & & & & & & & & & & & & \\
 & & & & 3\lambda & & & & & & & & & & & & & & \\
\hdashline
 & & 0 & & & & & & & 0 & & & & & & & & 0 & \\
\hdashline
 & & & & & & & & & & & & & & \lambda & & & & \\
 & & 0 & & & & & & & 0 & & & & & & \lambda & & & \\
 & & & & & & & & & & & & & & & & \lambda & & \\
 & & & & & & & & & & & & & & & & & \ddots & \lambda
\end{array}\right]
\end{array}$$

The matrix $\underline{A}$, in this orientation is the same, except that the diagonal submatrix of λ's is replaced by a diagonal matrix of ones due to multiplying by $\frac{1}{\lambda}$ from $N[\underline{X}_1'\underline{X}_1]^{-1}$.

To determine the generally rotated alias matrix we first pre and post multiply the combined moment matrix of the $\underline{X}_1$ and $\underline{X}_2$ independent variables by some orthogonal transforming matrix, that is,

$$N^{-1}\left[\begin{array}{cc|c} 1 & & \\ & \underline{H}' & \\ & & \underline{H}^{[2]\prime} \\ \hline & & \underline{H}^{[3]\prime} \end{array}\right]\left[\begin{array}{c|c} \underline{X}_1'\underline{X}_1 & \underline{X}_1'\underline{X}_2 \\ \hline \underline{X}_2'\underline{X}_1 & \underline{X}_2'\underline{X}_2 \end{array}\right]\left[\begin{array}{cc|c} 1 & & \\ & \underline{H} & \\ & & \underline{H}^{[2]} \\ \hline & & \underline{H}^{[3]} \end{array}\right]; \qquad (127)$$

where $\underline{H}$ is some arbitrary k x k orthogonal matrix, $\underline{H}^{[2]}$ is the second Schläflian matrix and $\underline{H}^{[3]}$ the third Schläflian matrix. To correspond to the definition of derived power vectors and Schläflians, see §8, the model is written so that the coefficient of the terms $x_i x_j$ is $\sqrt{2}$ and for the third order interaction terms $x_i^2 x_j$ and $x_i x_j x_k$ is $\sqrt{3}$. The second order Schläflian, written as before in abbreviated form, is

$$\underline{H}^{[2]} = \left[\begin{array}{c|c} \underline{\alpha} & \underline{\beta} \\ \hline \underline{\gamma} & \underline{\delta} \end{array}\right].$$

The third order Schläflian can be similarly written in abbreviated form as

$$\underline{H}^{[3]} = \left[\begin{array}{c|c|c} \underline{1} & \underline{2} & \underline{3} \\ \hline \underline{4} & \underline{5} & \underline{6} \\ \hline \underline{7} & \underline{8} & \underline{9} \end{array}\right] \qquad (128)$$

where the sub-matrices in $\underline{H}^{[3]}$ are partitioned after the k^{th} row and column and again after the $\frac{1}{2}(k + 1)(k + 2)$ row and column.

The generally rotated alias matrix, obtained from the expansion of equation (127) is

$$\text{Rotated } \underline{A} = \begin{bmatrix} 1 & & \\ & \underline{H}' & \\ & & \begin{matrix} \underline{\alpha}' & \underline{\gamma}' \\ \underline{\beta}' & \underline{\delta}' \end{matrix} \end{bmatrix} \underline{A} \begin{bmatrix} \underline{1} & \underline{2} & \underline{3} \\ \underline{4} & \underline{5} & \underline{6} \\ \underline{7} & \underline{8} & \underline{9} \end{bmatrix} \tag{129}$$

Remembering now that rotation cannot affect moments up to order four, the rows corresponding to the mean and linear terms in $\underline{A}$ remain constant so that, upon expanding (129)

$$\begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 11 \\ 22 \\ 33 \\ 44 \\ 55 \\ 12 \\ 13 \\ \vdots \\ 45 \end{array}
\begin{array}{ccccc|cccccccc|cccccc}
111 & 222 & 333 & 444 & 555 & 122 & 133 & 144 & 155 & 112 & 233 & \cdots & & 345 & 245 & 125 & 123 & 125 \ \cdots \\
\hline
 & & 0 & & & & & & 0 & & & & & & & 0 & & \\
\hline
3\lambda & & & & & \lambda & \lambda & \lambda & \lambda & & & & & & & & & \\
 & 3\lambda & & & & & & & & \lambda & \lambda & \lambda\ \lambda & & & & & & \\
 & & 3\lambda & & & & & & & & & & \lambda \text{ etc} & & & 0 & & \\
 & & & 3\lambda & & & & & & & & & & & & & & \\
 & & & & 3\lambda & & & & & & & & & & & & & \\
\hline
 & & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & & \\
 & & 0 & & & & & & 0 & & & & & & & 0 & & \\
 & & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & & \\
\hline
 & & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & & \\
 & & \underline{\delta}'[\underline{7}] & & & & & & \underline{\delta}'[\underline{8}] & & & & & & & \underline{\delta}'[\underline{9}] & & \\
 & & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & &
\end{array}$$

We note now that the interaction terms are biased by the unestimated third order effects.

One criteria advanced for determining the efficiency of any particular orientation of a design is to consider the sums of squares of the bias coefficients for each of the $\binom{k+2}{k}$ coefficients in the model. These sums of squares are given by the diagonal elements of $\underline{A}\ \underline{A}'$. (Box, G. E. P., Multifactor Designs of First Order, Biometrika, Vol. 39, 1952). The sums of squares of the alias coefficients for the interaction effects in any orientation are given by

$$\underline{\delta}' \left[\underline{7}\ \ \underline{8}\ \ \underline{9}\right] \begin{bmatrix} \underline{7}' \\ \underline{8}' \\ \underline{9}' \end{bmatrix} \underline{\delta} = \underline{\delta}' \underline{I}\, \underline{\delta} = \underline{\delta}' \underline{\delta}$$

Thus, since δ depends on the orientation, the magnitudes of the biases and their sums of squares also depend on the orientation of the design.