SIMPLEX-SUM DESIGNS: A CLASS OF SECOND ORDER ROTATABLE DESIGNS DERIVABLE FROM THOSE OF FIRST ORDER[1]

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1.0 Introduction. A functional relationship $\eta = g(\xi_1, \xi_2, \cdots, \xi_k) = g(\boldsymbol{\xi})$ is assumed to exist between a response η and k continuous variables $\xi_1, \xi_2, \cdots, \xi_k$. To elucidate certain aspects of this relationship measurements of η are to be made for each of N combinations of the levels of the variables

$$\boldsymbol{\xi}'_u = (\xi_{1u}, \xi_{2u}, \cdots, \xi_{ku}) \qquad u = 1, 2, \cdots, N.$$

The problem of experimental design considered is the choice of the *design matrix* **D** of N rows and k columns whose uth row is $\boldsymbol{\xi}'_u$ which specifies the levels of the variables to be used in each of the N trials. The design matrix can be regarded as specifying the coordinates of N *experimental points* in the k dimensional space of the variables. As mentioned for example in [1], [2], [3], and [4] a number of distinct problems can arise. Here we suppose as in [5] that the nature of the functional relationship $g(\boldsymbol{\xi})$ is unknown but that over a specific region R in the space of the variables $\xi_1, \xi_2, \cdots, \xi_k$ a polynomial of degree d, $f_d(\boldsymbol{\xi})$, adequately graduates the function $g(\boldsymbol{\xi})$ and the objective is to use the polynomial to estimate η within the region R. A design of order d is such that it allows the estimation of the polynomial $f_d(\boldsymbol{\xi})$. In this paper we shall be particularly concerned with the case of $d = 2$, that is with the fitting of a polynomial of second degree. Using specifically what is called a rotatable design, we shall develop a method of obtaining rotatable designs of second order from those of first order. In defining rotatable designs it may be appropriate here to discuss briefly why they are thought to be useful.

A general design may be expressed in terms of standardized variables, for which

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

and

$$N^{-1} \sum x_{iu}^2 = \lambda_2,$$

where λ_2 is a convenient constant. In actual application therefore the levels of the experimental variables ξ_i are given by $\xi_{iu} = S_i x_{iu} + \xi_{i0}$ where ξ_{i0} and S_i were suitably chosen so as to give appropriate location and spread to the design in the

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particular application. We shall suppose that the functional relationship is to be estimated by standard least squares.

A polynomial of degree one in the x's may be written

$$\eta_u = \sum_{i=0}^{k} \beta_i x_{iu}$$

where $x_{0u} = 1$, $u = 1, 2, \cdots, N$ or in matrix notation $\eta = \mathbf{X\beta}$ where $\mathbf{X}$ is a $N \times (k + 1)$ matrix

$$\mathbf{X} = [\mathbf{1} \vdots \mathbf{D}]$$

and $\mathbf{1}$ is an $N \times 1$ column vector with all its elements unity. Whether one's objective is to obtain minimum variance for the estimated linear coefficients, minimum volume of the confidence region for the coefficients, or minimum volume of the confidence cone for the direction of steepest ascent, one is led to the simple conclusion that the most desirable design is orthogonal, that is, it is such that $\mathbf{X'X} = N\mathbf{\Delta}$ where $\mathbf{\Delta}$ is a diagonal matrix with its first diagonal element equal to unity and its remaining diagonal elements equal to λ_2.

Often we are not particularly interested in estimating the individual coefficients β_i but in estimating the polynomial itself. Suppose a design has been carried out which allows us to fit the polynomial by least squares. Using the fitted polynomial the estimated response at the conditions $\mathbf{x}' = [x_1, x_2, \cdots, x_k]$ is denoted by $\hat{y}_\mathbf{x}$. If a polynomial of the degree assumed can exactly represent $g(\mathbf{x})$ then

$$E(\hat{y}_\mathbf{x}) = \eta_\mathbf{x}$$

and a measure of the accuracy of our estimation over the region of interest R is provided by $V(\hat{y}_\mathbf{x})$.

It is easy to show that a first order orthogonal design has the property that $V(\hat{y}_\mathbf{x})$ is a function of $\mathbf{x'x} = \sum x_i^2$ and λ_2 alone.

$$V(\hat{y}_\mathbf{x}) = \varphi(\mathbf{x'x}, \lambda_2)$$

For such a design therefore, this variance (and hence the reciprocal of the variance which can be regarded as a measure of the information supplied by the design about the response surface) is constant on circles, spheres or hyperspheres in the factor space, i.e., in the space of the variables $x_1, x_2, \cdots, x_k$. Designs which have the property of generating spherical variance contours are called *rotatable designs*. It is easily shown for first order designs that the converse proposition is true, that is in order to insure rotatability the design must be orthogonal. As is pointed out in [5] the criterion of orthogonality, which has a central place for the first order design, is not readily extendable to designs of higher order. We can, however, readily extend the property of rotatability to designs of higher order and it is found that in general for a design of order d it is possible to choose a design such that

$$V(\hat{y}) = \varphi(\mathbf{x'x}, \lambda_2, \lambda_4, \cdots \lambda_{2d})$$

where λ_i are constants at our choice.

To ensure the design is of this form it is only necessary to arrange that the moments of the design up to order $2d$ shall have certain values. For the case of second order designs with which we are specifically concerned

$$V(\hat{y}) = \varphi(\mathbf{x}'\mathbf{x}, \lambda_2, \lambda_4)$$

where λ_2 and λ_4 are at our choice. λ_2 is merely a scaling factor while λ_4 is chosen to give a satisfactory variance profile along a radius vector.

The problems for which the designs we are discussing have particular application are those where we are gaining knowledge of certain features of an unknown functional relationship by a sequential process in which any one "design" is only a single step. The results of each such step are used to more effectively plan the next group of observations.

At a particular stage we are interested in the behavior of the response function "in the neighborhood" R of some particular point P. We have in mind that the operability region O, that is the region in the space of the variables in which experiments could be conducted, is fairly extensive and that P is not close to the boundary of O. We suppose that the neighborhood of interest about P is a region R which nowhere reaches the boundary of O and that scales, metrics and transformations are chosen either implicitly or explicitly such that R is very approximately spherical and is centered at P.

The science of designing experiments is principally a convenient way of giving expression to prior information about the experimental situation which is currently in the experimenters mind and utilizing this information so as to generate further information most likely to be of value. The prior information is expressed in the choice of metrics, scales and transformations employed and is based on the experimenter's current feelings concerning the nature of the function under study. To the extent that the choices are poor, the extra information obtained about the nature of the function after the next set of observations have been completed, will be less than might otherwise have been obtained. This would mean that a sequence of such experiments, in which the information gained at each stage is utilized to design further more effective experiments, would be somewhat longer when prior information was less. This of course is to be expected and is a reflection of the fact that the apparent indeterminacy is a property of the experimental problem of exploring unknown functions itself, rather than of a particular technique for solving it. To demonstrate that some such rationale as the above is necessary one should remember that *any* set of experimental points distributed through the factor space such that $\mathbf{X}$ is of rank $k + 1$ provides a first order orthogonal design in some set of transformed x's.

The discussion so far has been based on the nature of the variance function $V(\hat{y}_{\mathbf{x}}) = E[\hat{y}_{\mathbf{x}} - E(\hat{y}_{\mathbf{x}})]^2$. In practice it would seldom if ever be true that the polynomial would provide an exact representation of the unknown function and in a more recent paper [2] this assumption has been dropped. Designs which minimize the mean square error $E(\hat{y}_{\mathbf{x}} - \eta_{\mathbf{x}})^2$ are considered instead. Now

$$E(\hat{y}_{\mathbf{x}} - \eta_{\mathbf{x}})^2 = V(\hat{y}_{\mathbf{x}}) + [E(\hat{y}_{\mathbf{x}}) - \eta_{\mathbf{x}}]^2$$

where the additional term on the right hand side may be called the squared bias. A general theorem in the above paper shows that if we are fitting a polynomial of degree d_1 over a region R when a polynomial of higher degree d_2 is necessary to give an exact representation, then the value of the squared bias averaged over the region, is minimized when the moments of the design points are the same as those of a uniform distribution over the region R. If it seems plausible in accordance with the previous discussion that the region of interest should be regarded as spherical then the optimum design to minimize average bias is also a particular rotatable design.

2.0. Outline. If we accept then that rotatable designs are of interest it becomes necessary to discover how they may be obtained in practice. First order rotatable designs are readily obtained (they are simply the orthogonal designs) but useful second order designs are less easy to derive. The method used here for obtaining second order rotatable designs from those of first order will now be outlined. In what follows we shall use n for the number of points in a first order design, and N for the size of a general or higher order derived design.

In the fitted first degree equation there are $k + 1$ constants, consequently at

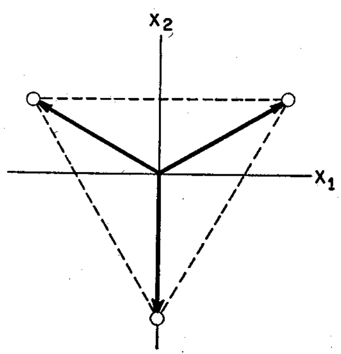

FIG. 1a. Two dimensional regular simplex

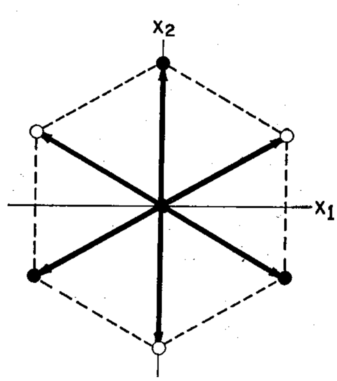

FIG. 1b. Generated second order rotatable design for two factors

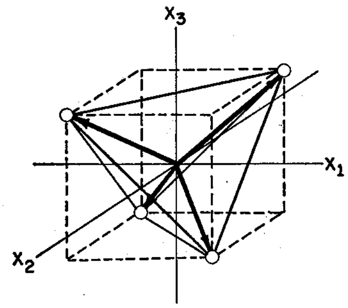

FIG. 2a. Three dimensional regular simplex

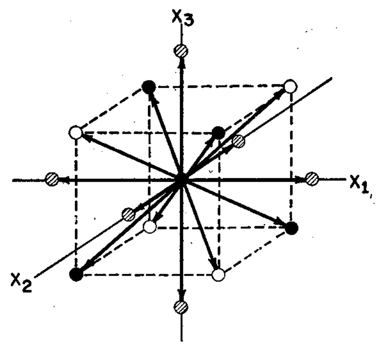

FIG. 2b. Generated second order rotatable design for three factors

least $k + 1$ observations must be made if the constants are to be separately estimable. Suppose the first order orthogonal (rotatable) design is used with the minimum number ($n = k + 1$) of experimental points. Then it is easily shown [6] that in the space of the x's these points lie at the vertices of a regular simplex. For example, if $k = 2$ the points are at the vertices of an equilateral triangle, if $k = 3$ at the corners of a regular tetrahedron. They can thus be called *first order simplex designs*. Now it can be observed that certain of the useful second order designs which have been found bear an interesting relation (illustrated for $k = 2$ and $k = 3$ in Figures 1 and 2) to the first order simplex designs. The three points at the vertices of an equilateral triangle in Figure 1a when joined to the origin at the center of the triangle, define three vectors. By adding these vectors two at a time we obtain a second equilateral triangle; by adding the vectors three at a time we obtain a center point. The original set of points plus the derived points generate the design shown in Figure 1b. This is the so-called hexagonal design which is known to be a second order rotatable design, [5]. The corresponding four vectors from the origin to the vertices of a tetrahedron shown in Figure 2a (a first order orthogonal or rotatable design) when added in all possible ways two at a time generate six further vectors passing through the midpoints of the edges of the tetrahedron, when added in all possible ways three at a time generate four vectors passing through the mid points of the faces of the original tetrahedron and when added four at a time generate a center point. If the lengths of the derived vectors are suitably chosen the resulting design coincides precisely with a previously derived second order rotatable design, namely the central composite rotatable design [5], [7]. These derived designs will be called *simplex-sum designs.*

In this paper we first demonstrate that the method suggested by these two examples for generating simplex-sum second order rotatable designs containing $2^n - 1$ points, from the first order rotatable simplex design containing $k + 1$ points, is a general one. For $k \geqq 5$ the number of points required by this method becomes large compared to the number of constants to be determined. A method is given for generating "fractions" and "replicated fractions" of the derived designs which have all the required properties and hence overcome this difficulty. Finally it is shown how the designs may be arranged in blocks so that they may be utilized in circumstances where insufficient homogeneous experimental material is available to complete the full quota of experimental runs.

To illustrate the method a second order rotatable design for seven variables is obtained, requiring only 66 experimental runs and only using three levels of each variable.

3.0. General Theory.

3.1. *Conditions for Rotatability.* We now define the design matrix **D** for the k standardized factors $x_1, x_2, \cdots, x_k$ as an $N \times k$ matrix whose uth row

$$\mathbf{x}_u' = (x_{1u}\, x_{2u} \cdots x_{ku})$$

defines the coded factor levels to be used in the uth of N experiments called for by the design. The general moment of the design will be denoted by

$$[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}] = N^{-1} \sum_{u=1}^{N} x_{1u}^{\alpha_1} x_{2u}^{\alpha_2} \cdots x_{ku}^{\alpha_k} .$$

and $\alpha = \sum \alpha_i$ will be called the order of the moment. The problem of finding rotatable designs is in essence one of finding configurations of points possessing the proper moments. It is in fact shown in [5] that when fitting the model

$$\eta = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j=i}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \sum_{j=i}^{k} \sum_{l=j}^{k} \beta_{ijl} x_i x_j x_l + \cdots$$

including all terms through degree d, a rotatable design will be obtained when the moments through order $2d$ are of the form

$$[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}] = \begin{cases} \lambda_\alpha \dfrac{\prod_{i=1}^{k} (\alpha_i)!}{2^{\alpha/2} \prod_{i=1}^{k} (\alpha_i/2)!}, & \text{all } \alpha_i \text{ even} \\ 0, & \text{any } \alpha_i \text{ odd,} \end{cases} \tag{3.1}$$

where λ_α is a constant for any design and α.

3.2. *Notation and Definition.* Consider a first order orthogonal (simplex) design in $k = n - 1$ variables with design matrix $\mathbf{D}_1$ and with $\sum_{u=1}^{n} x_{iu}^2$ set equal to n so that

$$\begin{bmatrix} \mathbf{1}' \\ \mathbf{D}_1' \end{bmatrix} [\mathbf{1}\ \mathbf{D}_1] = n\, \mathbf{I}_n .$$

It is conjectured that a second order rotatable design may be generated by using as design points the vectors obtained by taking all possible sums of the n rows of

$$\mathbf{D}_1 = \begin{bmatrix} \mathbf{x}_1' \\ \mathbf{x}_2' \\ \vdots \\ \mathbf{x}_u' \\ \vdots \\ \mathbf{x}_n' \end{bmatrix}$$

taken s at a time where $s = 1, 2, \cdots, k$. The problem thus reduces to one of finding the moments of a design matrix $\mathbf{D}$ derived in this way. We allow the vectors obtained by taking sums of s rows to be multiplied by a constant $a_s \geqq 0$. The constants $a_1, a_2, \cdots, a_k$ will be called *radius multipliers*. Then the N by k matrix $\mathbf{D}$ for the derived design is

$$\mathbf{D} = \begin{bmatrix} a_1 \mathbf{D}_1 \\ \hline a_2 \mathbf{D}_2 \\ \hline \vdots \\ \hline a_s \mathbf{D}_s \\ \hline \vdots \\ \hline a_k \mathbf{D}_k \end{bmatrix},$$

where $N = 2^n - 2$. Each $\mathbf{D}_s$ is an $\binom{n}{s}$ by k matrix whose rows consist of all possible sums of the rows of $\mathbf{D}_1$ taken s at a time. We omit for the moment the center point corresponding to $\mathbf{D}_{k+1}$ obtained when all n vectors are added together simultaneously. Since the columns of $\mathbf{D}_1$ are orthogonal to a vector of ones it follows that each vector obtained by summing rows s at a time is the negative of one obtained by summing rows $n - s$ at a time. The points in the factor space represented by $\mathbf{D}_s$ are, therefore, reflections through the origin of those represented by $\mathbf{D}_{n-s}$. (Of course, when n is even, $n - n/2 = n/2$ and half the rows of $\mathbf{D}_{n/2}$ are reflections of the other half.)

Let us define the *moment component* $[1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}]_s$ as $\binom{n}{s} N^{-1}$ times the specified moment of $\mathbf{D}_s$, i.e.,

$$[1^{\alpha_1} 2^{\alpha_2} \cdots k^{\alpha_k}]_s = \frac{1}{N} \sum_{1 \leqq u_1 < u_2} \sum \cdots \sum_{< u_s \leqq n} (x_{1u_1} + x_{1u_2} + \cdots + x_{1u_s})^{\alpha_1}$$
$$\cdot (x_{2u_1} + x_{2u_2} + \cdots + x_{2u_s})^{\alpha_2} \cdots (x_{ku_1} + x_{ku_2} + \cdots + x_{ku_s})^{\alpha_k}.$$

Then the corresponding moment for the entire design can be written

$$[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}] = \sum_{s=1}^{k} (a_s)^{\alpha}[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}]_s .$$

3.3. *Analogy to Sampling from a Finite Population.* The problem of finding expressions for $[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}]_s$ in terms of either the moments of D_1 or of $[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}]_1$ corresponds to that of finding the sampling moments of means (or totals) of samples of s drawn from a k-variate finite population of n elements. These moments can be derived by a method due to Tukey [8] and elaborated by Wishart [9], Hooke [10] and Robson [11]. The necessary derivations are given in [12], [13] and the results utilized for our purposes here.

The sampling analogy is readily seen if we consider a k-variate vector of means obtained by averaging a random sample of s k-variate vectors chosen from a population of n such vectors,

$$(\bar{x}_1, \bar{x}_2, \cdots, \bar{x}_k) = \frac{1}{s}\sum_{u=1}^{s} (x_{1u}, x_{2u}, \cdots, x_{ku}).$$

Then the joint sampling moments of these multivariate means are

$$\text{Ave}\,\{\bar{x}_1^{\alpha_1}\bar{x}_2^{\alpha_2} \cdots \bar{x}_k^{\alpha_k}\},$$

Ave denoting the average value of the indicated power product over all combinations of samples of s. These expressions can be used to obtain the moment components of any submatrix $\mathbf{D}_s$ since

$$[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}]_s = N^{-1}s^{\alpha}\binom{n}{s}\text{Ave}\,\{\bar{x}_1^{\alpha_1}\bar{x}_2^{\alpha_2} \cdots \bar{x}_k^{\alpha_k}\}.$$

Using this equality and the results in [12] (recalling $\sum_{u=1}^{n} x_{iu}^2 = n$, $i = 1, 2, \cdots, k$ here) the expressions for the required moment components are readily obtained and are shown in Table 1a for $n \geqq \alpha$. Table 1b gives the one case required here for $n < \alpha$ not covered by Table 1a.

3.4. *Form of Moment Components.* Tables 1a and 1b show the moment components in terms of a notation designed to simplify their use and to make clear their general pattern. Certain of the coefficients $C(s)$ have single subscripts while the remainder have double subscripts. The former are not multiplied by unrestricted moment components of $\mathbf{D}_1$ and hence are constant terms in the moment component equations for a given n and s. The latter however, are multiplied by $\mathbf{D}_1$ moment components such as $[i\,j^2]_1$, or combinations of $\mathbf{D}_s$ moment components and are therefore coefficients of quantities which will not in general be constant for different choices of i, j, k, l, m.

The values taken on by any coefficient function $C(s)$, when n is held constant, possess a symmetry with respect to s as a result of the reflection relationship between vectors in $\mathbf{D}_s$ and $\mathbf{D}_{n-s}$. Since one matrix is the negative of the other their respective components must differ only by the factor $(-1)^{\alpha}$ or

$$[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}]_s = (-1)^{\alpha}[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}]_{n-s} .$$

TABLE 1a

Summary of general moment components of $\mathbf{D}_s$, $(n \geqq \alpha)$

	General Formulas	Abbreviations
$[i]_s$	0	
$[ij]_s$	0	
$[i^2]_s$	$C_2(s)$	$C_2(s) = \binom{n-2}{s-1}\frac{n}{N}$
$[ijk]_s$	$C_{31}(s)[ijk]_1$	$C_{31}(s) = \frac{(n-2s)}{(n-2)}\binom{n-2}{s-1}$
$[ij^2]_s$	$C_{31}(s)[ij^2]_1$	
$[i^3]_s$	$C_{31}(s)[i^3]_1$	
$[ijkl]_s$	$C_{41}(s)[ijkl]_1$	$C_{41}(s) = \left[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\right]\binom{n-2}{s-1}$
$[ijk^2]_s$	$C_{41}(s)[ijk^2]_1$	
$[ij^3]_s$	$C_{41}(s)[ij^3]_1$	
$[i^2j^2]_s$	$C_4(s) + C_{41}(s)[i^2j^2]_1$	$C_4(s) = \binom{n-4}{s-2}\frac{n^2}{N}$
$[i^4]_s$	$3C_4(s) + C_{41}(s)[i^4]_1$	
$[ijklm]_s$	$C_{51}(s)[ijklm]_1$	$C_{51}(s) = (n-2s)\left[\frac{(n-3s)(n-4s) - 5n(s-1)}{(n-2)(n-3)(n-4)}\right]\binom{n-2}{s-1}$
$[ijkl^2]_s$	$C_{51}(s)[ijkl^2]_1 + C_{52}(s)[ijkl^2 \mid 2]_1$	$C_{52}(s) = \frac{(n-2s)}{(n-4)}\binom{n-4}{s-2}n$; $[ijkl^2 \mid 2]_1 = [ijk]_1$
$[i^5]_s$	$C_{51}(s)[i^5]_1 + 10C_{52}(s)[i^5 \mid 2]_1$	$[i^5 \mid 2]_1 = [i^3]_1$
$[i^2j^2k^2]_s$	$C_6(s) + C_{61}(s)[i^2j^2k^2]_1 + C_{62}(s)[i^2j^2k^2 \mid 2]_1 + 2C_{63}(s)[i^2j^2k^2 \mid 3]_1$	$C_6(s) = \binom{n-6}{s-3}\frac{n^3}{N}$; $C_{62}(s) = \left[\frac{n^2 + 3n - 6sn + 6s^2 - 4}{(n-4)(n-5)}\right]\binom{n-4}{s-2}n$

TABLE 1a—*Continued*

	General Formulas	Abbreviations
$[i^6]_s$	$15C_6(s) + C_{61}(s)[i^6]_1 + 15C_{62}(s)[i^6 \mid 2]_1 + 10C_{63}(s)[i^6 \mid 3]_1$	$C_{61}(s) = \binom{n-2}{s-1}\left[\frac{(n-2s)(n-3s)(n-4s)(n-5s)}{(n-2)(n-3)(n-4)(n-5)} - \frac{n(s-1)(16n^2 - 79sn + 11n + 86s^2 - 4s - 4)}{(n-2)(n-3)(n-4)(n-5)}\right]$ $C_{63}(s) = \left[\frac{n^2 - n - 4sn + 4s^2 + 4}{(n-4)(n-5)}\right]\binom{n-4}{s-2}N$ $[i^2j^2k^2 \mid 2]_1 = [i^2j^2]_1 + [i^2k^2]_1 + [j^2k^2]_1$ $[i^2j^2k^2 \mid 3]_1 = [ij^2]_1[ik^2]_1 + [i^2j]_1[jk^2]_1 + [i^2k]_1[j^2k]_1 + 2[ijk]_1^2$ $[i^6 \mid 2]_1 = [i^4]_1$ $[i^6 \mid 3]_1 = [i^3]_1^2$

TABLE 1b

Fourth order moment components of $\mathbf{D}_s$ *for* $n = 3$, $(n < \alpha)$

	General Formula	Abbreviation
$[ij^3]_s$	$C'_{41}(s)[ij^3]_1$	$C'_{41}(s) = \frac{s}{3!}\binom{3}{s}[2 - 7(s-1)]$
$[i^2j^2]_s$	$C'_4(s) + C'_{41}(s)[i^2j^2]_1$	$C'_4(s) = \frac{s}{3!}\binom{3}{s}(s-1)\frac{9}{N}$
$[i^4]_s$	$3C'_4(s) + C'_{41}(s)[i^4]_1$	

From Tables 1a and 1b we see that in general

$$(3.4)\quad \begin{aligned}[1^{\alpha_1}2^{\alpha_2}\cdots k^{\alpha_k}]_s &= b_\alpha C_\alpha(s) + C_{\alpha 1}(s)[1^{\alpha_1}2^{\alpha_2}\cdots k^{\alpha_k}]_1 \\ &+ b_{\alpha 2}C_{\alpha 2}(s)[1^{\alpha_1}2^{\alpha_2}\cdots k^{\alpha_k}\mid 2]_1 + \cdots + b_{\alpha p}C_{\alpha p}(s)[1^{\alpha_1}2^{\alpha_2}\cdots k^{\alpha_k}\mid p]_1,\end{aligned}$$

where the b_α values are zero or positive constants varying with the particular partition of $\alpha = (\alpha_1\alpha_2\cdots\alpha_k)$.

It is readily shown in general [13] and can be confirmed by direct substitution that $C_{\alpha i}(s) = (-1)^\alpha C_{\alpha i}(n - s)$.

4.0. Radius Multipliers and Rotatability. Having general formulas for the moment components contributed by each submatrix $\mathbf{D}_s$ of a derived design matrix $\mathbf{D}$, we now seek a suitable set of radius multipliers such that the moments of $\mathbf{D}$

$$(4.1)\quad [1^{\alpha_1}2^{\alpha_2}\cdots k^{\alpha_k}] = \sum_{s=1}^{k} a_s^\alpha[1^{\alpha_1}2^{\alpha_2}\cdots k^{\alpha_k}]_s$$

will fulfill the requirements for rotatability listed under (3.1).

By *even-order moments* we mean those for which $\alpha = \sum \alpha_i$ is even and by *odd-order moments* we mean those for which α is odd. In addition we call those moments for which *any* α_i is odd, *odd moments* and those for which all α_i are even, *even moments*. For rotatability all odd moments must be zero and all even moments of the same order must be specified multiples of each other.

From Table 1a we see that the moments $[i]$, $[ij]$ and $[i^2]$ of $\mathbf{D}$, will satisfy the rotatability requirements for any choice of radius multipliers since the corresponding odd moment components $[i]_s$ and $[ij]_s$ are identically zero and $[i^2]_s$ is constant for all i. The other moments however all involve "variable terms" $C_{\alpha i}(s)[\ ]_1$ and only in the case of the even moments is the constant term $b_\alpha C_\alpha(s)$ added to this variable function. The moment requirements will be generally satisfied only if the radius multipliers are so chosen that each "variable term" sums to zero in the expression for all $[1^{\alpha_1}2^{\alpha_2}\cdots k^{\alpha_k}]$. For odd moments this is obviously required. For the even moments it would otherwise be impossible to attain the required constant ratio between moments of the same order since the quantities $[\ ]_1$ in general change in their relationships, from one moment to another. The only further requirement for rotatability is that the constant terms, $b_\alpha C_\alpha(s)$, are in the required ratios.

Using the general form of $[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}]_s$ from (3.4) in (4.1) we have

$$
\begin{aligned}
[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}] &= \sum_{s=1}^{k} (a_s)^\alpha [1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}]_s \\
&= b_\alpha \sum_{s=1}^{k} (a_s)^\alpha C_\alpha(s) + [1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k}]_1 \cdot \sum_{s=1}^{k} (a_s)^\alpha C_{\alpha 1}(s) \\
&\quad + b_{\alpha 2}[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k} \mid 2]_1 \cdot \sum_{s=1}^{k} (a_s)^\alpha C_{\alpha 2}(s) \\
&\quad + \cdots + b_{\alpha p}[1^{\alpha_1}2^{\alpha_2} \cdots k^{\alpha_k} \mid p]_1 \cdot \sum_{s=1}^{k} (a_s)^\alpha C_{\alpha p}(s),
\end{aligned}
$$

where $b_\alpha C_\alpha(s)$ does not appear unless the moment is even and we require

$$\sum_{s=1}^{k} (a_s)^\alpha C_{\alpha i}(s) = 0, \qquad i = 1, 2 \cdots p.$$

Since we have seen previously that $C(s) = (-1)^\alpha C(n - s)$, then for all odd-order moments $C_{\alpha i}(s) = -C_{\alpha i}(n - s)$. We can say further, because of the factor $(n - 2s)$ in all such odd order moment coefficients, (Table 1a) that when α and k are both odd, $C_{\alpha i}(n/2) = C_{\alpha i}(k + 1/2) = 0$. Therefore as long as radius multipliers are selected such that $a_s = a_{n-s}$ *all* the odd-order moments will sum to zero for any value of a_s. Setting $m = k/2$ when k is even and $m = (k - 1)/2$when k is odd it then follows, for such a choice of radius multipliers, that

$$\sum_{s=1}^{k} (a_s)^\alpha C_{\alpha i}(s) = \sum_{s=1}^{m} (a_s)^\alpha [C_{\alpha i}(s) + C_{\alpha i}(n - s)] = 0 \text{ for all } i, \quad \alpha \text{ odd.}$$

We will call this type of solution for the radius multipliers, where $a_s = a_{n-s}$, a *symmetric solution.*

Having satisfied the odd-order moment requirements for rotatable designs of *any* order we must now find which symmetric solutions will also satisfy the requirements for even-order moments.

5.0. Second Order Requirements for Rotatability. For a design to be second order rotatable the even moments must have the following general form $[i^2] = \lambda_2$, $[i^2j^2] = \lambda_4$, $[i^4] = 3\lambda_4$ where λ_2 and λ_4 are constants at choice and the odd moments of order less than or equal to four must vanish.

It may be noted here that the addition of center points to a design matrix **D** does not change the general form of the moments since their only effect is to increase the denominator N.

5.1. *Application of Moment Requirements.* As noted previously in 4.0, the general second order moment $[i^2]$ places no restrictions on the choices of radius multipliers since

$$[i^2] = \sum_{s=1}^{k} (a_s)^2 C_2(s) = \frac{n}{N} \sum_{s=1}^{k} (a_s)^2 \binom{n-2}{s-1} = \lambda_2,$$

a constant for all values of i.

From Tables 1a and 1b it can be seen that the generalized moment component is obtained by letting the coefficient b_4 vanish for odd moments, and assume the values 3 and 1 for the even partitions of α, viz., (4) and (2,2). Hence

$$[i^{\alpha_1}j^{\alpha_2}k^{\alpha_3}l^{\alpha_4}]_s = b_4C_4(s) + C_{41}(s)[i^{\alpha_1}j^{\alpha_2}k^{\alpha_3}l^{\alpha_4}]_1$$

so that

$$[i^{\alpha_1}j^{\alpha_2}k^{\alpha_3}l^{\alpha_4}] = b_4\sum_{s=1}^{k} (a_s)^4C_4(s) + [i^{\alpha_1}j^{\alpha_2}k^{\alpha_3}l^{\alpha_4}]_1\sum_{s=1}^{k} (a_s)^4C_{41}(s).$$

In the previous section we showed that, for second order rotatability, we must have $\sum_{s=1}^{k} (a_s)^4C_{41}(s) = 0$ making

$$[i^{\alpha_1}j^{\alpha_2}k^{\alpha_3}l^{\alpha_4}] = b_4\sum_{s=1}^{k} (a_s)^4C_4(s).$$

This accomplished, all odd moments of order four would vanish with b_4 and

$$[i^2j^2] = \sum_{s=1}^{k} (a_s)^4C_4(s) = \lambda_4$$

$$[i^4] = 3\sum_{s=1}^{k} (a_s)^4C_4(s) = 3\lambda_4 .$$

Clearly any symmetric solution for the radius multipliers such that

$$\sum_{s=1}^{k} (a_s)^4C_{41}(s) = 0$$

will provide a rotatable design of the simplex-sum type.

5.2. *Standard Solution for Radius Multipliers.* We will now demonstrate that a solution holding for any k is obtained by letting

$$a_s = \binom{n-2}{s-1}^{-\frac{1}{4}}, \qquad s = 1, 2, \cdots k.$$

This solution for the radius multipliers involving the binomial coefficients will be denoted by $B_s^{-\frac{1}{4}}$ and referred to as the *standard solution.*

It is immediately evident that all odd order moments will be zero since the choice for the a_s provides a symmetric solution as defined earlier. Further

$$[i^2] = \sum_{s=1}^{k} \binom{n-2}{s-1}^{-\frac{2}{4}} \cdot \binom{n-2}{s-1}\frac{n}{N} = \frac{n}{N}\sum_{s=1}^{k} \binom{n-2}{s-1}^{\frac{1}{2}} = \lambda_2$$

and, for each i, $[i^2]$ equals n/N times the sum of the square roots of the binomial coefficients of order $n - 2$.

$$\begin{aligned}[i\,j\,k\,l] &= \sum_{s=1}^{n-1} \binom{n-2}{s-1}^{-\frac{4}{4}} \frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)} \binom{n-2}{s-1}[i\,j\,k\,l]_1 \\ &= \sum_{s=1}^{n-1} \frac{n^2 - 6sn + 6s^2 + n}{(n-2)(n-3)} [i\,j\,k\,l]_1 = \frac{[i\,j\,k\,l]_1}{(n-2)(n-3)}\,(0) = 0.\end{aligned}$$

Since the zero quantity in brackets is the expression $\sum a_s^4 C_{41}(s)$, common to all fourth order moments, we have

$$[i\, j\, k^2] = [i\, j^3] = 0,$$

$$[i^2 j^2] = \sum_{s=1}^{n-1} \binom{n-2}{s-1}^{-1} \binom{n-4}{s-2} \frac{n^2}{N} = \frac{n^2(n-1)}{6N} = \lambda_4 ,$$

$$[i^4] = \sum_{s=1}^{n-1} \binom{n-2}{s-1}^{-1} \binom{n-4}{s-2} \frac{3n^2}{N} = \frac{n^2(n-1)}{2N} = 3\,\lambda_4 .$$

5.3. *Second Order Rotatability for the Case $n = 3$.* For $k = 2$ ($n = 3$) the above demonstration does not apply since the fourth order moment formulas hold only for $n \geqq 4$ as noted previously. However by using the formulas in Table 1b, we can show that the above solution also applies here.

$$[i\, j^3] = \sum_{s=1}^{2} \binom{1}{s-1}^{-1} \frac{s}{3!} \binom{3}{s} [2 - 7\,(s-1)][i\, j^3]_1 = [i\, j^3]_1 - 5[i\, j^3]_1 .$$

Although apparently inconsistent with previous results this expression is zero because of a property of 3×3 matrices of the type $[\mathbf{1}\ \mathbf{x}_1\ \mathbf{x}_2]$ with orthogonal columns of equal vector length. Since we have already shown that a matrix of all rows taken s at a time is the negative of the matrix of sums taken $n - s$ at a time we have $\mathbf{D}_1 = -\mathbf{D}_2$ and $[i\, j^3]_1 = [i\, j^3]_2$. From the general moment formula for $n = 3$ we have $[i\, j^3]_2 = -5[i\, j^3]_1$ and hence $[i\, j^3]_1 = -5[i\, j^3]_1$ must vanish.

The moment

$$[i^2 j^2] = \sum_{s=1}^{2} \binom{1}{s-1}^{-1} \left\{ \frac{s}{3!} \binom{3}{s} [2 - 7\,(s-1)][i^2 j^2]_1 + (s-1)\, \frac{9}{N} \right\}$$

$$= [i^2 j^2]_1 - 5\, [i^2 j^2]_1 + \frac{9}{N} .$$

However since $[i^2 j^2]_1 = [i^2 j^2]_2$ and $[i^2 j^2]_2 = -5[i^2 j^2]_1 + 9/N$ we have $[i^2 j^2]_1 = 3/2N$, a constant for any matrix of this type. It then follows that $[i^2 j^2] = 2[i^2 j^2]_1 = 3/N = \lambda_4$ and similarly $[i^4] = 3\lambda_4$. Thus the moments are those of a rotatable design.

We have thus demonstrated that for $k \geqq 2$ a second order rotatable design can always be derived from the first order simplex design. It is possible to show however [13] that this method in its present form does not generate third order rotatable designs.

5.4. *Radius of Experimental Points.* As is illustrated in figures 1a and 1b for the case $k = 2$ and $k = 3$ the simplex-sum designs consist of subsets of vectors of experimental points corresponding to the rows of the submatrices $a_1\mathbf{D}_1$, $a_2\mathbf{D}_2$, $\cdots$, $a_k\mathbf{D}_k$. Geometrically these subsets are symmetrically oriented one to another in that the vectors for $a_2\mathbf{D}_2$ bisect the edges of the simplex defined by $a_1\mathbf{D}_1$, the vectors of $a_3\mathbf{D}_3$ pass symmetrically through the faces of the simplex defined by $a_1\mathbf{D}_1$ and so on. We can readily obtain an expression for r_s , the radius of the points in the sth subset. Denoting the uth row of $\mathbf{D}_s$ by $\mathbf{x}'_{su}$, $s = 2, 3, \cdots , k$

we have $\mathbf{x}'_{su} = \sum_{i=1}^{s} \mathbf{x}'_{u_i}$, where $\mathbf{x}'_{u_1}, \mathbf{x}'_{u_2}, \cdots, \mathbf{x}'_{u_s}$ is the uth set of s rows of the first order design matrix $\mathbf{D}_1$. Now since

$$[\mathbf{1}\ \mathbf{D}_1] = \begin{bmatrix} 1 & \mathbf{x}'_1 \\ 1 & \mathbf{x}'_2 \\ & \vdots \\ 1 & \mathbf{x}'_n \end{bmatrix}$$

and $[\mathbf{1}\ \mathbf{D}_1][\mathbf{1}\ \mathbf{D}_1]' = n\ \mathbf{I}_n$ we have

$$\mathbf{x}'_i\, \mathbf{x}_j = \begin{cases} n - 1 = k, & i = j \\ -1, & i \neq j. \end{cases}$$

The square of the length of the row vector $\mathbf{x}'_{su}$ is therefore

$$\mathbf{x}'_{su}\mathbf{x}_{su} = (\mathbf{x}'_{u_1} + \mathbf{x}'_{u_2} + \cdots + \mathbf{x}'_{u_s})(\mathbf{x}_{u_1} + \mathbf{x}_{u_2} + \cdots + \mathbf{x}_{u_s})$$

$$= s(n-1) + 2\binom{s}{2}(-1) = s(n-s).$$

Thus the radius of the experimental points in any submatrix $a_s\mathbf{D}_s$ is given by $r_s = a_s[s(n-s)]^{\frac{1}{2}}$, and since in a symmetric solution $a_s = a_{n-s}$, $r_s = r_{n-s}$.

For the particular set of radius multipliers of the standard solution $r_s = \binom{n-2}{s-1}^{-\frac{1}{4}}[s(n-s)]^{\frac{1}{2}}$. A summary of the radii for $k = 2$ through 8 of the standard solution rotatable designs is given in Table 2.

TABLE 2

Radii of experimental points for standard solution rotatable designs

k	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8
2	1.41	1.41						
3	1.73	1.68	1.73					
4	2.00	1.86	1.86	2.00				
5	2.24	2.00	1.92	2.00	2.24			
6	2.45	2.11	1.95	1.95	2.11	2.45		
7	2.65	2.21	1.97	1.89	1.97	2.21	2.65	
8	2.83	2.30	1.98	1.84	1.84	1.98	2.30	2.83

5.5. *Singularity and Near Singularity of Moment Matrices.* A set of points can have the moments of a rotatable design but be impractical as a design since it leads to a singular moment matrix. The singularity arises from a dependency between the columns in the $\mathbf{X}$ matrix for the b_0 and quadratic terms, $b_{11}, b_{22}, \cdots, b_{kk}$. The situation is easily remedied, however, by the addition of center points to the design matrix. The moment matrix is singular [5] when the standardized fourth moment constant λ'_4 achieves the value $\lambda'_4 = \lambda_4/(\lambda_2)^2 = k/(k+2)$, implying that the design points all lie on the same hypersphere [14]. For the

TABLE 3

Comparison of λ_4' to its singular value for standard solution designs

k	$\frac{k}{(k+2)}$	λ_4'
2	.500	.500
3	.600	.601
4	.667	.670
5	.714	.724
6	.750	.769
7	.778	.811
8	.800	.850

designs arising from the standard solution for a_s we have

$$\lambda_4' = \frac{n^2(n-1)}{6N}\left[\frac{n\sum_{s=1}^{n-1}\binom{n-2}{s-1}^{\frac{1}{2}}}{N}\right]^{-2} = \frac{(n-1)(2^n-2)}{6\left[\sum_{s=1}^{n-1}\binom{n-2}{s-1}^{\frac{1}{2}}\right]^2}$$

where we have used $N = 2^n - 2$, i.e., no center points having been added. The value for λ_4' is equal to the singular value $k/(k+2)$ when $k = 2$ and remains close to the singular value as k increases, as is shown in Table 3.

Since the addition of center points has no effect on the moments except to change N we see that the addition of N_0 center points will change λ_4' by a factor of $(2^n - 2 + N_0)/(2^n - 2)$. In practice sufficient center points were added to provide a satisfactory profile for the variance function $V(\hat{y}_x)$ taken along a radius vector. Denoting the distance from the center of the design by $\rho = (\mathbf{x}'\mathbf{x})^{\frac{1}{2}}$ it is suggested in general in [5] that sufficient points be added so that $V(\hat{y}_x)$ at $\rho = 0$ is equal to that at $\rho = (\lambda_2)^{\frac{1}{2}}$. Such an arrangement causes the variance to be approximately uniform over the important range $\rho = 0$ to $\rho = (\lambda_2)^{\frac{1}{2}}$. These designs will be said to attain "uniform variance".

6.0. Additional Second Order Rotatable Simplex-Sum Designs. The standard solution for a_s affords a set of rotatable designs for all $k \geqq 2$. When $k \geqq 5$ however, the number of experiments required by the standard solution becomes excessive. Fortunately, for such values of k smaller *reduced designs* are possible.

6.1. *Solution Space of Radius Multipliers.* We have shown in Section 4 that for second order rotatability we must find values for a_s, $s = 1, 2, \cdots, k$, such that $\sum a_s^3 C_{31}(s) = 0$ and $\sum a_s^4 C_{41}(s) = 0$ where $C_{31}(s)$ and $C_{41}(s)$ are the coefficients of the moment components of $\mathbf{D}_1$ (Tables 1a and 1b). When those values are found it was shown that the other moment requirements were automatically satisfied.

To state these requirements in a more convenient form for our present problem let us define the vectors

$$\mathbf{a}' = (a_1\, a_2 \cdots a_s \cdots a_k),$$

$$\mathbf{a}_3' = (a_1^3\, a_2^3 \cdots a_s^3 \cdots a_k^3),$$

$$\mathbf{a}_4' = (a_1^4\, a_2^4 \cdots a_s^4 \cdots a_k^4),$$

$$\mathbf{C}_{31}' = (C_{31}(1)\ C_{31}(2) \cdots C_{31}(s) \cdots C_{31}(k)),$$

$$\mathbf{C}_{41}' = (C_{41}(1)\ C_{41}(2) \cdots C_{41}(s) \cdots C_{41}(k)).$$

The requirements for second order rotatability are therefore $\mathbf{C}_{31}'\mathbf{a}_3 = 0$ and $\mathbf{C}_{41}'\mathbf{a}_4 = 0$. If we choose values of $\mathbf{a}_s$, such that $a_s = a_{n-s}$, we have shown previously that $\mathbf{C}_{31}'\mathbf{a}_3 = 0$. Therefore, calling any vectors $\mathbf{a}_3$ and $\mathbf{a}_4$ which are derived from symmetric solutions, *symmetric vectors*, we may further simplify our problem to that of finding all symmetric vectors $\mathbf{a}_4$ such that $\mathbf{C}_{41}'\mathbf{a}_4 = 0$. We must also add the restrictions of course, that all the elements of $\mathbf{a}_4$ are greater than zero.

The restriction of symmetry on the vector $\mathbf{a}_4$ has the effect of confining its values to an m dimensional subspace for which $m = k/2$, if k is even and $m = (k + 1)/2$, if k is odd. This is evident since $\mathbf{a}_4$ has exactly m elements which can be varied independently, the remaining $k - m$ elements then being determined by the relationship $a_s = a_{n-s}$. The elements of $\mathbf{C}_{41}$ are symmetric in a corresponding way as was shown earlier. Hence for convenience we might consider $\mathbf{a}_4$ and $\mathbf{C}_{41}$ as two m-dimensional vectors and use the fact that $m - 1$ independent vectors can be found orthogonal to any vector in m-space. Thus if we find $m - 1$ independent solutions to the equation $\mathbf{C}_{41}'\mathbf{a}_4 = 0$ they will form a basis for the solution space of all possible vectors satisfying this equation, that is of all vectors in the $m - 1$ space orthogonal to $\mathbf{C}_{41}$. Since the elements of $\mathbf{C}_{41}$ are of mixed sign it is clear that solution vectors can be found which fall in the positive 2^k-drant.

6.2. *Specific Solutions.* We will now obtain the $m - 1$ basis vectors $\boldsymbol{\Upsilon}_1, \boldsymbol{\Upsilon}_2, \cdots \boldsymbol{\Upsilon}_{m-1}$ for $k = 3, 4, \cdots 8$, selecting them to contain the maximum number of zero elements possible. Where zero's can be introduced, the equivalent designs will involve fewer points than the standard solution since any submatrix with a zero radius multiplier, may be eliminated from $\mathbf{D}$ without altering the moments. All other designs, resulting from the orthogonality relationship, can be derived from these basis vectors by taking linear combinations

$$\mathbf{a}_4 = d_1\boldsymbol{\Upsilon}_1 + d_2\boldsymbol{\Upsilon}_2 + \cdots + d_{m-1}\boldsymbol{\Upsilon}_{m-1},$$

where the d_i's are any constants such that $\mathbf{a}_4 \geqq \mathbf{0}$.

It will be recalled from the discussion of the standard solution that the two factor design is an anomaly in that its rotatability does not result from the orthogonality relationship. For $k = 2$, $\mathbf{C}_{41}'\mathbf{a}_4 \neq 0$ and hence a specific solution does not follow in the usual way. When $k = 3$, $m = 2$ and hence only one solution, the standard solution, is available, $(\boldsymbol{\Upsilon}_1 = \mathbf{a}_4)$. Similarly when $k = 4$, $m =$

2 so that for $k \leqq 4$ the standard solution is unique. When $k = 5$ however then $m = 3$ and two independent solutions $\mathbf{\Upsilon}_1$ and $\mathbf{\Upsilon}_2$ are possible. Specifically

$$\mathbf{C}'_{41}\mathbf{\Upsilon}_i = (1 \quad -2 \quad -6 \quad -2 \quad 1)\mathbf{\Upsilon}_i = 0,$$

and here for the first time we can obtain reduced designs. Two suitable basis vectors are

$$\mathbf{\Upsilon}'_1 = (1 \quad 0 \quad \tfrac{1}{3} \quad 0 \quad 1),$$
$$\mathbf{\Upsilon}'_2 = (1 \quad \tfrac{1}{2} \quad 0 \quad \tfrac{1}{2} \quad 1),$$

whence

$$\mathbf{a}' = (1 \quad 0 \quad 3^{-\frac{1}{2}} \quad 0 \quad 1),$$
$$\mathbf{a}' = (1 \quad 2^{-\frac{1}{2}} \quad 0 \quad 2^{-\frac{1}{2}} \quad 1).$$

The arrangement employing $\mathbf{\Upsilon}_1$ omits $a_2\mathbf{D}_2$ and $a_4\mathbf{D}_4$ while that employing $\mathbf{\Upsilon}_2$ omits $a_3\mathbf{D}_3$ from the design.

When $k = 6$, then $m = 3$ and the relationship

$$\mathbf{C}'_{41}\mathbf{\Upsilon}_i = (1 \quad -1 \quad -8 \quad -8 \quad -1 \quad 1)\mathbf{\Upsilon}_i = 0,$$

is satisfied by

$$\mathbf{\Upsilon}'_1 = (1 \quad 1 \quad 0 \quad 0 \quad 1 \quad 1),$$
$$\mathbf{\Upsilon}'_2 = (1 \quad 0 \quad \tfrac{1}{8} \quad \tfrac{1}{8} \quad 0 \quad 1).$$

When $k = 7$, then $m = 4$ and

$$\mathbf{C}'_{41}\mathbf{\Upsilon}_i = (1 \quad 0 \quad -9 \quad -16 \quad -9 \quad 0 \quad 1)\mathbf{\Upsilon}_i = 0$$

is satisfied by

$$\mathbf{\Upsilon}'_1 = (1 \quad 0 \quad \tfrac{1}{9} \quad 0 \quad \tfrac{1}{9} \quad 0 \quad 1),$$
$$\mathbf{\Upsilon}'_2 = (1 \quad 0 \quad 0 \quad \tfrac{1}{8} \quad 0 \quad 0 \quad 1),$$
$$\mathbf{\Upsilon}'_3 = (0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0).$$

When $k = 8$, then $m = 4$ and

$$\mathbf{C}'_{41}\mathbf{\Upsilon}_i = (1 \quad 1 \quad -9 \quad -25 \quad -25 \quad -9 \quad 1 \quad 1)\mathbf{\Upsilon}_i = 0,$$

which is satisfied by

$$\mathbf{\Upsilon}'_1 = (1 \quad 0 \quad \tfrac{1}{9} \quad 0 \quad 0 \quad \tfrac{1}{9} \quad 0 \quad 1),$$
$$\mathbf{\Upsilon}'_2 = (1 \quad 0 \quad 0 \quad \tfrac{1}{25} \quad \tfrac{1}{25} \quad 0 \quad 0 \quad 1),$$
$$\mathbf{\Upsilon}'_3 = (0 \quad 1 \quad \tfrac{1}{9} \quad 0 \quad 0 \quad \tfrac{1}{9} \quad 1 \quad 0).$$

A fourth reduced design can be derived from the vector

$$\mathbf{a}_4 = \mathbf{\Upsilon}_2 - \mathbf{\Upsilon}_1 + \mathbf{\Upsilon}_3 = (0 \quad 1 \quad 0 \quad \tfrac{1}{25} \quad \tfrac{1}{25} \quad 0 \quad 1 \quad 0).$$

TABLE 4

Radius multipliers for some second order rotatable designs

k	Design	Radius Multipliers								No. of Experimental Points[a]			
										Simplex-Sum Designs		Composite Designs	
		a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	Radial Points	Center Points[b]	Radial Points	Center Points[b]
2	Std.	1	1							6	3	8	5
3	Std.	1	.8409	1						14	6	14	6
4	Std.	1	.7598	.7598	1					30	14	24	7
5	Std.	1	.7071	.6389	.7071	1				62	24		
	Υ_2	1	.8409	0	.8409	1				42	10		
	Υ_1	1	0	.7598	0	1				32	8	26	6
6	Std.	1	.6687	.5623	.5623	.6687	1			126	38		
	Υ_2	1	0	.5946	.5946	0	1			84	16		
	Υ_1	1	1	0	0	1	1			56	13	44	9
7	Std.	1	.6389	.5081	.4729	.5081	.6389	1		254	59		
	Υ_1	1	0	.5774	0	.5774	0	1		128	21		
	Υ_2	1	0	0	.5946	0	0	1		86	15		
	Υ_3	0	1	0	0	0	1	0		56	10	78	14
8	Std.	1	.6150	.4671	.4111	.4111	.4671	.6150	1	510	90		
	Υ_2	1	0	0	.4472	.4472	0	0	1	270	26		
	Υ_3	0	1	.5774	0	0	.5774	1	0	240	0		
	Υ_1	1	0	.5774	0	0	.5774	0	1	186	28	80	13

[a] The "Composite Design" values refer to the composite second order rotatable designs derived in [5] and are included for comparative purposes. Half replicates of the cube portion are used for $k = 5$, 6 and 7 and one quarter replicate for $k = 8$.

[b] Number of centerpoints required for "uniform variance" within $\rho = (\lambda_2)^{\frac{1}{2}}$.

A summary of the radius multipliers used to obtain the standard solution designs (B_s^{-1}) and the specific solution designs derived from the basis vectors, is given in Table 4. It can be seen that only the reduced designs will be practical in most instances when $k > 4$ since N increases rapidly. Also included in the table are the number of center points required to attain "uniform variance".

In order to produce a design using Table 4, it is only necessary to select a suitable matrix $\mathbf{D}_1$ and by taking all sums of rows s at a time, for each s of the non-zero a_s values, generate the required $\mathbf{D}_s$ matrices. Multiplication of $\mathbf{D}_s$ by a_s will then give the coordinates of the design points. An example is given in Section 9.

7.0. Replication. If it should be desired to replicate certain subsets of the derived matrices this can easily be done by making suitable adjustments to the radius multipliers. We will only consider the case where symmetric replication is used (i.e., $\mathbf{D}_s$ and $\mathbf{D}_{n-s}$ are replicated equally), thus ensuring that a symmetric solution for the radius multipliers can be found.

If we replicate a particular pair of submatrices $\mathbf{D}_s$ and $\mathbf{D}_{n-s}$ ν_s times, the elements $C_{31}(s)$, $C_{41}(s)$, $C_{31}(n - s)$ and $C_{41}(n - s)$ will be multiplied by ν_s and the moment equations will become

$$\sum_{s=1}^{k} \nu_s(a_s)^3 C_{31}(s) = 0,$$

$$\sum_{s=1}^{k} \nu_s(a_s)^4 C_{41}(s) = 0.$$

The first equation will still be negatively symmetric and will therefore be satisfied by any symmetric vector. The second equation will be satisfied if the new $\nu_s(a_s)^4$ equal the old $(a_s)^4$. Thus

$$a_s(\mathbf{D}_s \text{ replicated } \nu_s \text{ times}) = a_s(\text{unreplicated})/(\nu_s)^{\frac{1}{4}},$$

and a similar relation holds for radii.

For example, consider the standard solution for $k = 3$, and various patterns of replication. (We will always have $\nu_1 a_1^4 = 1$, $\nu_2 a_2^4 = \frac{1}{2}$, $\nu_3 a_3^4 = 1$.) Table 5 shows some results.

TABLE 5

The standard solution with $k = 3$ and various replication patterns

Pattern	Replications			Radius Multipliers			Radii		
	ν_1	ν_2	ν_3	a_1	a_2	a_3	r_1	r_2	r_3
1	1	1	1	1	$2^{-\frac{1}{4}}$	1	1.73	1.68	1.73
2	2	1	2	$2^{-\frac{1}{4}}$	$2^{-\frac{1}{4}}$	$2^{-\frac{1}{4}}$	1.45	1.68	1.45
3	1	8	1	1	2^{-1}	1	1.73	1.00	1.73

8.0. Blocking. When an experiment cannot be run under homogeneous conditions it is usually desirable to block the trials in such a way that the coefficients can be estimated efficiently while the error is confined to the magnitude of variation within blocks. We will assume that under the experimental conditions peculiar to any block the relationship of the response to the factors remains unchanged with the exception of a shift in level. Following the development in [5] then we assume the expected value of the uth experimental observation is represented by the model

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

where

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

and β_{0w} is the level parameter for the wth block, z_{wu} is a dummy variable assuming the value unity when the uth experiment falls in block w and zero otherwise, n_w is the number of observations in the wth block (including center points) and $N = \sum_{w=1}^{m} n_w$.

8.1. *Orthogonal Blocking–Rotatable Designs.* It is shown in [5] that orthogonal blocking is obtained when the within block moment components of the design (denoted by $[i^{\alpha_1}j^{\alpha_2}]_{bw}$) have the following properties:

1. $$[i]_{bw} = \frac{1}{N} \sum_{u}^{n_w} x_{iu} = 0,$$

2. $$[i\,j]_{bw} = \frac{1}{N} \sum_{u}^{n_w} x_{iu}\, x_{ju} = 0, \qquad i \neq j$$

3. $$[i^2]_{bw} = \frac{1}{N} \sum_{u}^{n_w} x_{iu}^2 = \frac{n_w}{N} \lambda_2, \qquad w = 1, 2 \cdots m,$$

where $\sum_{u}^{n_w}$ indicates summation over the n_w design points within the wth block.

The blocking arrangements we consider here will be called submatrix blocking schemes since they utilize the submatrices $a_1\mathbf{D}_1, a_2\mathbf{D}_2, \cdots, a_k\mathbf{D}_k$, or combinations of them, as blocks. From the general formulas for the moment components of these submatrices it is clear that they individually satisfy the first two conditions above. To individually satisfy the third condition however it is necessary that the quantities a_s^2 be such that their ratios are rational numbers. Instead of using the submatrices themselves as the basis for blocking, combinations of these submatrices can be employed. If the a_s are such that they allow blocks to be formed which yield a ratio of $[i^2]_{bw}/\lambda_2$ which is equal to a rational number then orthogonal blocks can be obtained. Table 6 shows some blocking arrangements which are derived in this way for the designs in Table 4.

In general the *individual* submatrices can not be employed as blocks without sacrificing either orthogonal blocking or rotatability. It is naturally most reasonable to sacrifice rotatability since clearly we only require an approximately "symmetric distribution" of information. Unfortunately when the conditions for rotatability are relaxed in this way the general inverse of the resulting matrix is not easily written down. When an electronic computer is used in the analysis of data however this presents little difficulty. The radius multipliers required for orthogonal blocking differ little from those required for rotatability and the resulting designs are thus nearly rotatable. Table 7 provides these values of a_s together with the "uniform variance" number of center points for each sub-matrix block.

8.2. *Non-orthogonal Blocking of the Rotatable Designs.* An alternative would be to retain rotatability but to accept slightly non-orthogonal blocking. From the

TABLE 6

Summary of orthogonal blocking schemes for rotatable designs of Table 4

k	Design	Block	Number of points in Block from Submatrix								Total No. of Points in Block		
			a_1D_1	a_2D_2	a_3D_3	a_4D_4	a_5D_5	a_6D_6	a_7D_7	a_8D_8	Sans Center Points	Center Points Added[a]	Grand Total (n_w)
2	Std.	1	3								3	2	5
		2		3							3	2	5
3	none												
4	Std.	1	5	10							15	7	22
		2			10	5					15	7	22
5	Υ_2	1	6	15							21	5	26
		2				15	6				21	5	26
6	Std.	1	7	21	35						63	19	82
		2				35	21	7			63	19	82
	Υ_2	1	7		35						42	8	50
		2				35		7			42	8	50
	Υ_1	1	7	21							28	6	34
		2					21	7			28	6	34
	Υ_1	1	7								7	(0)	7
		2		21							21	(14)	35
		3					21				21	(14)	35
		4						7			7	(0)	7
7	Υ_1	1	8		56						64	10	74
		2					56		8		64	10	74
	Υ_3	1		28							28	5	33
		2						28			28	5	33
	Υ_1	1	8								8	(4)	12
		2			56						56	(4)	60
		3					56				56	(4)	60
		4							8		8	(4)	12
8	Std.	1	9	36	84	126					255	45	300
		2					126	84	36	9	255	45	300
	Υ_2	1	9			126					135	13	148
		2					126			9	135	13	148
	Υ_3	1		36	84						120	0	120
		2						84	36		120	0	120

TABLE 6—*Continued*

k	Design	Block	Number of points in Block from Submatrix								Total No. of Points in Block		
			$a_1\mathbf{D}_1$	$a_2\mathbf{D}_2$	$a_3\mathbf{D}_3$	$a_4\mathbf{D}_4$	$a_5\mathbf{D}_5$	$a_6\mathbf{D}_6$	$a_7\mathbf{D}_7$	$a_8\mathbf{D}_8$	Sans Center Points	Center Points Added[a]	Grand Total (n_w)
	Υ_1	1	9		84						93	14	107
		2						84		9	93	14	107
	Υ_2	1	9								9	(9) (10)	18 19
		2				126					126	(0) (7)	126 133
		3					126				126	(0) (7)	126 133
		4								9	9	(9) (10)	18 19
	Υ_3	1		36							36	(48)	84
		2			84						84	(0)	84
		3						84			84	(0)	84
		4							36		36	(48)	84
	Υ_1	1	9								9	(4)	13
		2			84						84	(7)	91
		3						84			84	(7)	91
		4								9	9	(4)	13

[a] Those values not in brackets are the number of centerpoints required for "uniform variance" and can be replaced by any other number evenly distributed between blocks. The values in brackets also provide uniform variance but can not be changed freely without loss of orthogonality.

point of view of computational difficulty this approach turns out to be much the simpler, while the loss of information due to the slight non-orthogonality in blocking is small. In reference [15] the moment conditions are given which the points within the individual blocks must satisfy in order to retain rotatability. In particular it is shown that these conditions are met by any blocks which satisfy conditions 1 and 2 in Section 8.1 and hence by the submatrices $a_1\mathbf{D}_1$, $a_2\mathbf{D}_2$, $\cdots$, $a_k\mathbf{D}_k$ whether or not they are augmented with center points. Thus when only condition 3 is violated in blocking a rotatable design the variance-covariance matrix of the response surface coefficients (adjusted for the block effects) retains the form necessary to give "spherical" variance contours. The form also readily lends itself to providing a general explicit solution for the normal equations. The estimates of the regression coefficients for any such arrangement are given below where we let $\bar{y}_w$ denote the average of the observations in block w and use the notation

$$\{iy\} = \sum_{u=1}^{n} y_u , \qquad \{iy\} = \sum_{u=1}^{n} x_{iu} y_u , \qquad \{ijy\} = \sum_{u=1}^{n} x_{iu} x_{ju} y_u ,$$

$$A_\alpha^{-1} = 2\lambda_4 \left[(k+2)\lambda_4 - kN \sum_{w}^{m} [i^2]_{bw}^2 / n_w \right]$$

to give

$$b_0 = N^{-1}\left[\{0y\} - 2A_\alpha\lambda_4\lambda_2\left(\sum_i^k \{iiy\} - kN\sum_w^m [i^2]_{bw}\bar{y}_w\right)\right],$$

$$b_{ii} = N^{-1}A_\alpha\left[\{iiy\}A_\alpha^{-1} + \left(N\sum_w^m \frac{[i^2]_{bw}^2}{n_w} - \lambda_4\right)\sum_i^k \{iiy\} - 2\lambda_4 N\sum_w^m [i^2]_{bw}\bar{y}_w\right],$$

$$b_i = (\lambda_2 N)^{-1}\{iy\},$$

$$b_{ij} = (\lambda_4 N)^{-1}\{ijy\}.$$

The variances and covariances are

$$V(b_0) = 2\sigma^2\lambda_4 N^{-1}A_\alpha\left[(k+2)\lambda_4 - k\left(N\sum_w^m \frac{[i^2]_{bw}^2}{n_w} - \lambda_2^2\right)\right],$$

$$V(b_i) = \sigma^2(N\lambda_2)^{-1}, \qquad V(b_{ij}) = \sigma^2(N\lambda_4)^{-1},$$

$$V(b_{ii}) = \sigma^2 N^{-1}A_\alpha\left[(k+1)\lambda_4 - (k-1)N\sum_w^m \frac{[i^2]_{bw}^2}{n_w}\right],$$

$$\text{Cov}\,(b_0 b_{ii}) = -2\sigma^2\lambda_4\lambda_2 N^{-1}A_\alpha, \qquad \text{Cov}\,(b_{ii}b_{jj}) = \sigma^2 N^{-1}A_\alpha\left[N\sum_w^m \frac{[i^2]_{bw}^2}{n_w} - \lambda_2^2\right].$$

It will be noted that the variances of b_i and b_{ij} are not affected by non-orthogonal blocking but the variance of the constant term b_0 and the quadratic terms b_{ii} are affected. In [15] it is shown that the loss of information introduced by the small degree of non-orthogonality is small.

The variance function from which the variance of an estimated value $\hat{y}$ can

TABLE 7

Radius multipliers and center points for orthogonal nearly rotatable submatrix blocking

k	Original Design	D_1		D_2		D_3		D_4		D_5		D_6		D_7		D_8	
		a_1	n_{10}	a_2	n_{20}	a_3	n_{30}	a_4	n_{40}	a_5	n_{50}	a_6	n_{60}	a_7	n_{70}	a_8	n_{80}
3	Standard	1	2	.8165	2	1	2										
4	Standard	1	3	.7638	4	.7638	4	1	3								
5	Standard	1	4	.7071	5	.6583	6	.7071	5	1	4						
	Υ_2	1	1	.8238	4	0	0	.8238	4	1	1						
	Υ_1	1	1	0	0	.7868	6	0	0	1	1						
6	Standard	1	6	.6679	8	.5547	5	.5547	5	.6679	8	1	6				
	Υ_2	1	4	0	0	.5954	4	.5954	4	0	0	1	4				
7	Standard	1	8	.6455	12	.5164	8	.4776	3	.5164	8	.6455	12	1	8		
	Υ_2	1	3	0	0	0	0	.5992	9	0	0	0	0	1	3		
8	Standard	1	12	.6172	20	.4690	13	.4140	0	.4140	0	.4690	13	.6172	20	1	12

readily be calculated is

$$V(\hat{y}) = \sigma^2 N^{-1} A_\alpha \left\{ 2(k+2)\lambda_4^2 - 2k\lambda_4 \left(N \sum_w^m \frac{[i^2]_{bw}^2}{n_w} - \lambda_2^2 \right) \right.$$
$$+ 2\lambda_4 \lambda_2^{-1} \left[(k+2)\lambda_4 - \left(kN \sum_w^m \frac{[i^2]_{bw}^2}{n_w} + 2\lambda_2^2 \right) \right] \rho^2$$
$$\left. + \left[(k+1)\lambda_4 - (k-1) N \sum_w^m \frac{[i^2]_{bw}^2}{n_w} \right] \rho^4 \right\}.$$

9.0. A Convenient Reduced Design for $k = 7$. The design derived from the basis vector, Υ_3 for the seven factor design in Section 6.2, has several interesting features which will be discussed here. Since it requires but 56 points (plus center points) to estimate the 36 coefficients of a seven factor second degree polynomial, it is extremely efficient. The comparable central composite design [5]

TABLE 8

Seven factor second order rotatable design in three levels

½D₂							½D₆						
1	1	0	1	0	0	0	−1	−1	0	−1	0	0	0
1	0	1	0	1	0	0	−1	0	−1	0	−1	0	0
1	0	0	0	0	1	1	−1	0	0	0	0	−1	−1
0	1	1	0	0	1	0	0	−1	−1	0	0	−1	0
0	1	0	0	1	0	1	0	−1	0	0	−1	0	−1
0	0	1	1	0	0	1	0	0	−1	−1	0	0	−1
0	0	0	1	1	1	0	0	0	0	−1	−1	−1	0
1	0	0	0	0	−1	−1	−1	0	0	0	0	1	1
1	0	−1	0	−1	0	0	−1	0	1	0	1	0	0
0	1	0	0	−1	0	−1	0	−1	0	0	1	0	1
0	1	−1	0	0	−1	0	0	−1	1	0	0	1	0
0	0	0	1	−1	−1	0	0	0	0	−1	1	1	0
0	0	−1	1	0	0	−1	0	0	1	−1	0	0	1
1	−1	0	−1	0	0	0	−1	1	0	1	0	0	0
0	0	1	−1	0	0	−1	0	0	−1	1	0	0	1
0	0	0	−1	1	−1	0	0	0	0	1	−1	1	0
0	−1	1	0	0	−1	0	0	1	−1	0	0	1	0
0	−1	0	0	1	0	−1	0	1	0	0	−1	0	1
0	0	0	−1	−1	1	0	0	0	0	1	1	−1	0
0	0	−1	−1	0	0	1	0	0	1	1	0	0	−1
0	−1	0	0	−1	0	1	0	1	0	0	1	0	−1
0	−1	−1	0	0	1	0	0	1	1	0	0	−1	0
−1	1	0	−1	0	0	0	1	−1	0	1	0	0	0
−1	0	1	0	−1	0	0	1	0	−1	0	1	0	0
−1	0	0	0	0	1	−1	1	0	0	0	0	−1	1
−1	0	0	0	0	−1	1	1	0	0	0	0	1	−1
−1	0	−1	0	1	0	0	1	0	1	0	−1	0	0
−1	−1	0	1	0	0	0	1	1	0	−1	0	0	0

requires 78 points (plus center points). The vector of radius multipliers that defines this design is $\mathbf{a}' = (0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0)$ and thus utilizes the points specified by the matrices $\mathbf{D}_2$ and $\mathbf{D}_6$ only.

In seven dimensions it is possible to find a matrix $\mathbf{D}_1$, giving the coordinates of a regular simplex, which involves only the two levels -1 and $+1$, for each factor. Consequently $\mathbf{D}_2$ and $\mathbf{D}_6$ need only involve three factor levels. Furthermore $\mathbf{D}_2$ and $\mathbf{D}_6$ provide orthogonal blocks.

The 8×8 matrix $[\mathbf{1}\ \mathbf{D}_1]$ which can be used to generate this design is

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \end{bmatrix}$$

Its squared vector length is eight, as required, and all rows and columns are orthogonal.

The derived matrices $\frac{1}{2}\mathbf{D}_2$ and $\frac{1}{2}\mathbf{D}_6$ are shown in Table 8. Since multiplication by a constant is permissible, we will define our derived design matrix $\mathbf{D}$ therefore as

$$\mathbf{D} = \begin{bmatrix} \frac{1}{2} & \mathbf{D}_2 \\ \frac{1}{2} & \mathbf{D}_6 \end{bmatrix}$$

The singularity of the moment matrix of this design is readily detectable by noting that all the points lie on a hypersphere of radius $(3)^{1/2}$ and hence center points must be added to make all coefficients separately estimable. The addition of ten such points will produce a design having the "uniform variance" property.

For this design (and whenever nonorthogonal blocking does not complicate the normal equations) the regression coefficients and their variances are easily obtained from the general solutions for rotatable designs given in [5].

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