SIMPLEX-SUM DESIGNS

A CLASS OF SECOND ORDER ROTATABLE DESIGNS

DERIVABLE FROM THOSE OF FIRST ORDER

by

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TABLE OF CONTENTS

TABLE OF CONTENTS (continued)

LIST OF TABLES

Appendix B

1.0 INTRODUCTION

The objective of many experimental programs is to elucidate the relationship between a measurable characteristic of a material or process (η) and a set of continuously variable factors ($X_1, X_2, \ldots, X_k$) suspected of influencing its behavior. An insight into the problem can frequently be obtained by fitting a hypothesized model $\eta = f(\underline{X})$ to experimental data by least squares. The geometric representation of the fitted function has been called the response surface and much has been written in recent years describing the philosophy and technique of obtaining an estimate of the surface and of locating optimum points thereon.

Often lacking a more fundamental model, it is assumed that within the limited range of the experiment the unknown function can adequately be represented by a limited number of terms of its Maclaurin's Series expansion. We thus assume the approximation

$$\eta = \beta_o + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \sum_{j=i}^{k} \beta_{ij} X_i X_j + \sum_{i=1}^{k} \sum_{j=i}^{k} \sum_{\ell=j}^{k} \beta_{ij\ell} X_i X_j X_\ell + \cdots$$

where the β's are unknown constants proportional to the partial derivatives evaluated at the origin. A model utilizing all terms through degree d in the above expansion is called a d-th order model.

Designs used in response surface work are called d-th order designs if they allow estimation of all coefficients up to and including those of a d-th order model. In discussing designs it is convenient to think of the set of k factor levels called for by an experiment as the elements of a row vector and hence as a point in a k dimensional factor space. The set of N experiments called for by a design are then specified by an N x k design matrix D, each row of which defines the levels of an experiment and is one of the N points in the design configuration in the factor space. For convenience and to generalize the designs the levels of the independent variables are coded such that the origin of the new variables (x_1, x_2, ..., x_k) lies at the centroid of the design points and a suitable scaling convention is employed to make the design units uniform for all factors. From the first convention we have $\sum_u x_{iu} = 0$ and the second is usually effected by letting $\sum_u x_{iu}^2/N = \lambda_2$, a constant for all i.

Any design providing unique estimates of the coefficients in the model could be used but certain configurations of points offer distinct advantages. In response surface work the primary emphasis is, by definition, on the estimate of the surface and its variance. However, at the inception of an experimental program there is usually no knowledge of the orientation or shape of the surface relative to the axes of the factors and it is therefore desirable to use designs which are independent of this state of ignorance. With this objective in mind designs have been found for which the variance of an estimate is constant at all points equidistant from the origin of the design, i.e. for which the variance is independent of direction. These are called rotatable designs since the variances of both the estimated response and the individual coefficients are invariant under orthogonal rotation of the design in the factor space. In this way the design is unprejudiced by the arbitrary characteristics of the surface relative to the orientation of the factor axes. While rotatability is a function of the scaling convention adopted, the variance contours will be spherical in those units appearing to the experimenter as most reasonable at the time the experiment is conducted, i.e. units based on the relative experimental variation in each factor.

First order rotatable designs are obtained when the columns of the design matrix D are orthogonal to each other and to a vector of ones. The first order model, which fits a planar surface to the data, contains k + 1 constants to be estimated and consequently requires a minimum of k + 1 points. When this minimum number is used it has been shown by Box in (5) that the design points will be at the vertices of a regular simplex in the factor space. When k = 2 the points lie at the vertices of an equilateral triangle, when k = 3 at the vertices of a regular tetrahedron and in general are one orientation of the unique set of k + 1 vectors of equal length forming equal angles with each other in k space.

Second order rotatable designs are obtained when more restrictive moment conditions are satisfied (where a general moment is defined as $\sum_u x_{1u}^{\alpha_1} x_{2u}^{\alpha_2} \ldots x_{ku}^{\alpha_k}/N$), and in two instances were found to bear an interesting relationship to the simplex designs just described. When k = 2 the points at the vertices of a hexagon provide the basis for a second order rotatable design. Now if the vectors of the equilateral triangle, forming the first order rotatable design, are added in pairs the three derived vectors, when taken in conjunction with the original three, will produce the vertices of a hexagon. If the original vectors are added three at a time they will provide a center point which is required to make the set of points a usable design of full rank.

When k = 3 a similar construction exists. A set of six vectors can be derived from those at the vertices of the tetrahedron by forming sums of all possible vector pairs. These vectors will pass through the mid points of the edges of the tetrahedron. Formation of all possible sums of three vectors will yield four derived vectors each passing through the mid point of a face of the tetrahedron. Again a center point is obtained by adding all four vectors. When the length of the three sets of vectors are suitably chosen (by scalar multiplication of each set) a previously derived second order rotatable design is obtained. This is the composite design which can be represented, as described above, by the row vectors $\underline{x}'_u = (x_{1u}\ x_{2u}\ x_{3u})$, $u = 1,2,\ldots,14$. The design consists of the six points denoted by $(\pm 2^{3/4}\ 0\ \ 0)$, $(0\ \ \pm 2^{3/4}\ 0)$, $(0\ \ 0\ \ \pm 2^{3/4})$ and the eight points at the vertices of a cube which can be represented by all permutations of sign of the vector $(\pm 1\ \pm 1\ \pm 1)$. To this basic set of fourteen a certain number of points at the origin (0 0 0) are usually added.

If we chose the original tetrahedron to be in that orientation in which the vertices have the coordinates of a fraction of the 2^3 factorial $(-1\ -1\ -1)$, $(1\ \ 1\ -1)$, $(1\ -1\ \ 1)$ and $(-1\ \ 1\ \ 1)$, then the relationship is readily seen. The six vectors corresponding to the axial points are those generated by adding the vectors two at a time, while the vectors corresponding to the second mating tetrahedron forming the remaining points of the cube (the second half-replicate) are those obtained by adding the basic vectors three at a time. To obtain the proper vector length for the axial points it can be seen that all six derived vectors must be multiplied by the constant $2^{-1/4}$.

This dissertation is concerned first with establishing the generality of the connection between first and second order rotatable designs, that is demonstrating that the design matrix of a first order rotatable design can always be used to produce the design matrix of a second order rotatable design (or designs). Secondly it is concerned with the possibility of generating third order rotatable designs in this manner, and finally with a description of the properties of the designs which evolved.

It was found that a class of second order rotatable designs, labelled simplex-sum designs can always be generated by taking as design points the vectors obtained by forming all possible sums of the k + 1 rows of any minimum first order rotatable design matrix, and multiplying the derived vectors by suitable constants. Third order rotatable designs however did not materialize from this straightforward approach. As a by-product of the investigation, sampling moments for means of finite multivariate orthogonal populations were derived which may find use in other applications. The blocking properties of simplex-sum designs were thoroughly investigated and a general theorem proved, for any second order rotatable design, concerning requirements necessary to retain rotatability when non-orthogonal blocking is used.

2.0 REVIEW OF LITERATURE

2.1 Surface Fitting

The literature on the general subject of response surface fitting has been reviewed extensively during the past several years, the most recent complete compilation appearing in a doctoral dissertation by Carter in 1957 (15). Papers covered there will be but briefly touched upon here, emphasis being put on the more recent publications.

In 1941 Hotelling (24) devised procedures that had certain optimal properties for locating the maximum of a function within a predetermined region of one and two dimensional factor spaces. A sequential scheme was then provided by Friedman and Savage (22) in 1947 for locating an optimum, when more than one factor is involved, based on the classical approach of varying one factor at a time.

The Box-Wilson paper (13) appeared in 1951 as the first of a sequence of papers by Box and associates and outlined an approach and viewpoint which set the stage for much of the work that followed. In this paper a sequential "steepest ascent" procedure is outlined for locating the region of a maximum and composite designs were then proposed for estimating the coefficients of a quadratic model within this region. In 1952 Box (5) showed that orthogonal designs were most efficient for estimating the constants of a first order model.

A review and discussion of the work published in this general field by 1953 was given by Anderson (3).

In 1954 several papers were published, one (6) of a general expository nature by Box on the methodology and philosophy on surface fitting, another by Box, Hader and Hunter (9) on the effects of having assumed an inadequate model showing biases existing in both the estimates and sums of squares, and a paper by Box and Hunter (10) concerned with setting a confidence region on the solution of a set of simultaneous equations with random coefficients (the latter problem being that encountered in solving for the stationary point of a fitted quadratic surface). De La Garza (20) also published a paper in 1954 showing that when only one independent variable was involved, designs for fitting polynomials of degree d involving more than d+1 points were equivalent from the standpoint of the variance-covariance matrix, to a design calling for exactly d+1 points.

A paper published in 1957 (12) by Box and Hunter, (having in large part appeared in 1954 in mimeograph form (11)), made explicit the definition of rotatable designs establishing the necessary and sufficient moment conditions for models of any order. Second order rotatable designs were found and blocking procedures provided for them. An approximate confidence region for the maximum was given based on the earlier Box and Hunter paper (10) but which was considerably simplified through the use of rotatable designs. The work of Wallace (29) was cited as a means of finding approximate limits which are easier to compute.

Box and Youle in 1955 (14) indicated how an empirical response surface approach could lead to an understanding of the fundamental theory of a process or reaction. It is shown how reduction to canonical variables can be of assistance in such an investigation.

Third order rotatable designs were discussed in 1956 by Gardiner, Grandage and Hader (23) for two, three and four factor experiments. These designs were based upon the regular figures and several were of a type allowing sequential fitting of the second and third order model.

Attention was given to blocking composite designs by DeBaun in 1956 (17). In a short paper he indicated the biases encountered in non-orthogonal blocking and gave an orthogonal blocking scheme for the five factor composite rotatable design. This material was later covered more generally in (12).

An extensive investigation of response surface designs for two factors was made by Carter in 1957 (15). The connection between the individual degrees of freedom of the standard factorial analysis and response surface coefficients was demonstrated. First and second order rotatable designs were given which are not necessarily based on regular figures. A procedure was given whereby any set of points could be completed into a first order rotatable design by adding two additional points. It was also shown how second order designs could be constructed from the various classes of first order designs described, by adding four additional points. A general theorem was proved showing necessary and sufficient conditions which must be satisfied for a combination of rotatable sets of order d-1 to be a rotatable set of order d.

In 1958 Bose and Draper (4) found infinite classes of second order rotatable designs for from three to seven factors. Infinite classes of sequential third order rotatable designs were also described. All previous second and third order designs were shown to belong to these classes. It was shown that the necessary and sufficient condition for the moment matrix of second and third order designs to be singular is for all design points to lie on a hypersphere in the factor space. The designs discussed are constructed from sets of points whose odd moments vanish and whose combination into rotatable designs depends upon satisfying certain "excess" functions defining the required relationship among the fourth order moments for second order designs together with sixth order moments for third order designs. In 1958 Draper (21) added a four factor third order rotatable design by using the same approach.

DeBaun in 1958 (18) and 1959 (19) described three factor three level second order designs for response surface work which are often of interest to an experimenter who finds it expensive or inconvenient to create more than the minimum number of factor levels. With one exception these designs are in the nearly rotatable class, having variance contours which approximate spheres.

A general method for producing three level designs in k factors was presented by Box and Behnken in 1958 (7) giving examples of both rotatable and nearly rotatable second order designs. These designs are generated by utilizing the combinatorial properties of partially balanced incomplete block designs. A means of characterizing the departure of the variance contours from sphericity was obtained for nearly rotatable designs.

Also in 1958 van der Vaart (28) proved some results on estimation of latent roots of a symmetric matrix relevant to the representation of a response surface as a quadratic function. He showed that estimates of the lowest latent root are biased downward and those of the largest root are biased upward. This implies that the latent roots will be of different signs unduly often and that hence there is a tendency to obtain surfaces that are of the minimax type more often than is correct. This result has some experimental verification.

A different departure on designs for exploring response surfaces was taken by Box and Draper in 1958 (8). Designs were sought which were optimal when both the random experimental error and the bias introduced by failure of the model were considered. The paper was principally concerned with the situation where a first order model was assumed when the true function was quadratic. It was found that the best design under typical conditions was one that minimized bias alone, ignoring variance. In this situation, at least, the optimal design is first order rotatable since it was shown that the requirement implies orthogonality. An interesting general result found here was that for any d_1-th order model which was used in place of the correct model of order d_2 the average bias is minimized by making the moments of order $d_1 + d_2$ and less equal to those of a uniform distribution over the region of interest.

2.2 Sampling Moments

In developing the moments of the experimental designs it was helpful to use a tool due to Tukey (26,27) which he entitled bracket notation. In two papers techniques were developed to simplify the algebra involved in computing moments and k-statistics of finite populations. A correspondence is established between k-statistics and brackets and rules for manipulating the two are provided. While considerable work has been done by others utilizing k-statistics, only the bracket notation was applicable here and we will not digress beyond this field of interest. One example of the use of these methods was given by Wishart (31) who considered univariate populations.

3.0 GENERAL THEORY

3.1 Conditions for Rotatability

To formalize the discussion in Section 1.0 we shall adhere to the notation in (12) and define the design matrix D for the k factors $x_1, x_2, \ldots, x_k$ as an N x k matrix whose u-th row

$$\underline{x}_u' = (x_{1u}\ x_{2u}\ \ldots x_{ku})$$

defines the coded factor levels to be used in the u-th of N experiments called for by the design. The general moment of the design will be denoted by the symbol $[1^{\alpha_1}\ 2^{\alpha_2}\ \ldots k^{\alpha_k}]$ where

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

The sum of the powers, denoted by $\alpha = \sum \alpha_i$ will be called the order of the moment.

Recalling that a design is called rotatable (12) when the function defining the variance at an arbitrary point $\underline{x}$ in the factor space depends only upon $\rho = \sqrt{\underline{x}'\underline{x}}$, the distance of the point from the origin, and that this function is completely determined by the moments of the design matrix, it is clear that 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 (12) that when fitting the model

$$\eta = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j=i}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \sum_{j=i}^{k} \sum_{\ell=j}^{k} \beta_{ij\ell} x_i x_j x_\ell + \ldots$$

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

$$[1^{\alpha_1}\ 2^{\alpha_2}\ \ldots\ k^{\alpha_k}] = \lambda_\alpha \frac{\prod_{i=1}^{k} (\alpha_i)!}{2^{\alpha/2} \prod_{i=1}^{k} (\alpha_i/2)!}, \quad \text{all } \alpha_i \text{ even}$$

$$= 0 \qquad \text{any } \alpha_i \text{ odd},$$

where λ_α is a constant for any design and α.

3.2 Notation and Definition

If we define the minimum k factor first order rotatable design matrix as D_1, an n x k matrix (letting $n = k+1$) possessing the minimum number of rows needed to estimate the constants of a first order model, then the moment conditions will be satisfied if the matrix obtained by augmenting D_1 on the left by a column of unit elements is proportional to an orthogonal matrix, i.e.,

$$\begin{bmatrix} \underline{1}' \\ D_1' \end{bmatrix} [\underline{1}\ D_1] = n\ I_n.$$

Starting with D_1 then it is conjectured that rotatable designs may be generated by taking all possible sums of the n rows of

$$D_1 = \begin{bmatrix} \underline{x}_1' \\ \underline{x}_2' \\ \vdots \\ \underline{x}_u' \\ \vdots \\ \underline{x}_n' \end{bmatrix}$$

taken s at a time where $s = 1, 2, \ldots k$. The problem thus reduces to one of finding the moments of a design matrix D derived in this way. We shall allow the moments to be modified by multiplication of the set of vectors obtained by taking sums of s rows by a constant $a_s \geq 0$. These constants $a_1, a_2, \ldots, a_k$ will be called radius multipliers since this scalar multiplication in effect determines the distance of each point from the center of the design.

We shall consider the derived N by k design matrix D as partitioned into the k submatrices

$$D = \begin{bmatrix} a_1 D_1 \\ \hline a_2 D_2 \\ \hline \vdots \\ \hline a_s D_s \\ \hline \vdots \\ \hline a_k D_k \end{bmatrix},$$

where $N = 2^n - 2$. Each D_s is an $\binom{n}{s}$ by k matrix whose rows consist of all possible sums of the rows of D_1 taken s at a time and a_s is the corresponding radius multiplier. We shall omit for the moment the case where all n vectors are added together simultaneously, i.e., the center point corresponding to D_{k+1}.

The moments of D can be subdivided into k component parts, one contributed by each of the submatrices, $D_1, D_2, \ldots, D_k$. Summing the rows of D_1 we have

$$\underline{x}_1' + \underline{x}_2' + \ldots + \underline{x}_s' + \ldots + \underline{x}_n' = \underline{0}'$$

where $\underline{0}'$ denotes a null vector, since

$$\sum_u x_{iu} = 0 \qquad \text{for each } i,$$

and hence

$$\underline{x}_1' + \underline{x}_2' + \ldots + \underline{x}_s' = -(\underline{x}_{s+1}' + \underline{x}_{s+2}' + \ldots + \underline{x}_n').$$

Thus we see 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 D_s are, therefore, reflections through the origin of those represented by D_{n-s}. (Of course, when n is even, $n - n/2 = n/2$ and half the rows of $D_{n/2}$ are reflections of the other half.

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

$$[1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}]_s = \frac{1}{N} \sum_{1 \leq u_1} \sum_{< u_2} \cdots \sum_{< u_s \leq n} (x_{1u_1} + x_{1u_2} + \ldots + x_{1u_s})^{\alpha_1}$$

$$\cdot (x_{2u_1} + x_{2u_2} + \ldots + x_{2u_s})^{\alpha_2} \ldots (x_{ku_1} + x_{ku_2} + \ldots + x_{ku_s})^{\alpha_k}.$$

Then the corresponding moment for the entire design can be written

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

where $\alpha = \sum_{i=1}^{k} \alpha_i$ following the notation adopted previously.

3.3 Analogy to Sampling from a Finite Population

The problem of finding expressions for $[1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}]_s$ in terms of either the moments of D_1 or of $[1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}]_1$ corresponds to that of finding the sampling moments for 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 (26,27) and elaborated by Wishart (31) for the univariate case. This method has been extended here in part, to cover the multivariate case. The details of this work are covered in the appendix. Appendix A extends the definition of "brackets" as defined in (26) to the multivariate case. It is shown that these expressions possess the same property as their univariate counterparts. Namely, if we use "Ave" to denote averaging over all possible samples of s from a population of n, and $\sum^{\neq}$ denotes summation over the unequal subscripts i, j, ..., q, then

$$\text{Ave}\left\{\sum^{s}{}^{\neq}\frac{x_{1i}^{p_1}\,x_{2j}^{p_2}\cdots x_{mq}^{p_m}}{s(s-1)\,\ldots\,(s-m+1)}\right\} = \sum^{n}{}^{\neq}\frac{x_{1i}^{p_1}\,x_{2j}^{p_2}\cdots x_{mq}^{p_m}}{n(n-1)\,\ldots\,(n-m+1)}$$

or, using bracket notation instead,

$$\text{Ave}\left\{\left\langle x_1^{p_1}, x_2^{p_2}, \ldots, x_m^{p_m}\right\rangle\right\} = \left\langle x_1^{p_1}, x_2^{p_2}, \ldots, x_m^{p_m}\right\rangle'$$

where the vector $(x_{1u}\ x_{2u}\ \ldots\ x_{mu})$ is one of s m - variate observations drawn from n such and a prime superscript added to a bracket denotes substitution of population values for sample values.

In Appendix B this property is used to derive the general expressions for the joint sampling moments of multivariate means. The moments are the average values of power products of the k coordinate means,

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

of samples of $s < n$ k - variate vectors drawn from a finite population of n such vectors. These values, which can be written in bracket notation as

$$\text{Ave}\left\{\langle x_1\rangle^{\alpha_1}\cdot\langle x_2\rangle^{\alpha_2}\ldots\langle x_k\rangle^{\alpha_k}\right\}$$

since

$$\langle x_i\rangle = \frac{\sum_{u=1}^{s}x_{iu}}{s},$$

are then used to obtain the moment components $[1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}]_s$ of the matrices D_s.

The following equality holds

$$[1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}]_s = N^{-1} s^{\alpha} \binom{n}{s} \quad \text{Ave} \quad \left\{ \langle x_1 \rangle^{\alpha_1} \ \langle x_2 \rangle^{\alpha_2} \ \ldots \ \langle x_k \rangle^{\alpha_k} \right\}$$

since we can regard the n row vectors of D_1 as a k - variate population and we require the moments of sums of vectors taken s at a time. The factor s^{α} is required since we want moments of sums, not means, and the factor $\binom{n}{s}$ to give the total moment of all $\binom{n}{s}$ terms. These results are summarized in general form in the appendix and are given in Table 1 for the particular case of interest here, that of standardized vector length equal to $\sqrt{n}$. The exception to Table 1a (p. 17) follows in Table 1b.

Table 1b. Fourth order moment components of D_s for n = 3, (n < α)

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

3.4 Form of Moment Components

Table 1 shows the moment components in terms of a notation designed to simplify their use in succeeding sections, and which makes clear their general pattern. The coefficient functions C(s) are of two types. Those with single subscripts are not multiplied by unrestricted moment components of D_1 and hence they are constants in the moment component equations for a given n and s. The coefficient functions involving two subscripts,

Table 1a. Summary of general moment components of D_s, $(n \geq \alpha)$

	General Formulas	Abbreviations
$[i]_s$	0	
$[ij]_s$	0	
$[i^2]_s$	$C_2(s)$	$C_2(s) = \binom{n-2}{s-1}\frac{n}{N}$
$[ijk]_s$	$C_{31}(s)[ijk]_1$	$C_{31}(s) = \frac{(n-2s)}{(n-2)} \binom{n-2}{s-1}$
$[ij^2]_s$	$C_{31}(s)[ij^2]_1$	
$[i^3]_s$	$C_{31}(s)[i^3]_1$	
$[ijkl]_s$	$C_{41}(s)[ijkl]_1$	$C_{41}(s) = [\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}] \binom{n-2}{s-1}$
$[ijk^2]_s$	$C_{41}(s)[ijk^2]_1$	
$[ij^3]_s$	$C_{41}(s)[ij^3]_1$	
$[i^2j^2]_s$	$C_4(s) + C_{41}(s)[i^2j^2]_1$	$C_4(s) = \binom{n-4}{s-2}\frac{n^2}{N}$
$[i^4]_s$	$3C_4(s) + C_{41}(s)[i^4]_1$	
$[ijklm]_s$	$C_{51}(s)[ijklm]_1$	$C_{51}(s) = (n-2s)\ [\frac{(n-3s)(n-4s) - 5n(s-1)}{(n-2)(n-3)(n-4)}] \binom{n-2}{s-1}$
$[ijkl^2]_s$	$C_{51}(s)[ijkl^2]_1 + C_{52}(s)[ijkl^2\|2]_1$	$C_{52}(s) = \frac{(n-2s)}{(n-4)}\binom{n-4}{s-2}n;$ $[ijkl^2\|2]_1 = [ijk]_1$
$[i^5]_s$	$C_{51}(s)[i^5]_1 + 10C_{52}(s)[i^5\|2]_1$	$[i^5\|2]_1 = [i^3]_1$
$[i^2j^2k^2]_s$	$C_6(s) + C_{61}(s)[i^2j^2k^2]_1 + C_{62}(s)[i^2j^2k^2\|2]_1 + 2C_{63}(s)[i^2j^2k^2\|3]_1$	$C_6(s) = \binom{n-6}{s-3}\frac{n^3}{N};$ $C_{62}(s) = [\frac{n^2 + 3n - 6sn + 6s^2 - 4}{(n-4)(n-5)}] \binom{n-4}{s-2}n$
$[i^6]_s$	$15C_6(s) + C_{61}(s)[i^6]_1 + 15C_{62}(s)[i^6\|2]_1 + 10C_{63}(s)[i^6\|3]_1$	$C_{61}(s) = [\frac{(n-2s)(n-3s)(n-4s)(n-5s) - n(s-1)(16n^2-79sn+11n+86s^2-4s-4)}{(n-2)(n-3)(n-4)(n-5)}]\binom{n-2}{s-1}$
		$C_{63}(s) = [\frac{n^2 - n - 4sn + 4s^2 + 4}{(n-4)(n-5)}] \binom{n-4}{s-2}N$
		$[i^2j^2k^2\|2] = [i^2j^2]_1 + [i^2k^2]_1 + [j^2k^2]_1$
		$[i^2j^2k^2\|3]_1 = [ij^2]_1[ik^2]_1 + [i^2j]_1[jk^2]_1 + [i^2k]_1[j^2k]_1 + 2[ijk]_1^2$
		$[i^6\|2]_1 = [i^4]_1$
		$[i^6\|3]_1 = [i^3]_1^2$

however, are multiplied by D_1 moment components such as $[i\ j^2]_1$, or combinations of 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 D_s and D_{n-s}. Since one matrix is the negative of the other their respective components must differ only by the factor $(-1)^{\alpha}$ or

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

From Table 1 we see that in general

$$[1^{\alpha_1}\ 2^{\alpha_2} \ldots k^{\alpha_k}]_u = b_{\underline{\alpha}}C_{\alpha}(u) + C_{\alpha 1}(u)[1^{\alpha_1}\ 2^{\alpha_2} \ldots k^{\alpha_k}]_1$$
$$+ b_{\underline{\alpha}2}C_{\alpha 2}(u)[1^{\alpha_1}\ 2^{\alpha_2} \ldots k^{\alpha_k} | 2]_1 + \ldots + b_{\underline{\alpha}p}C_{\alpha p}(u)[1^{\alpha_1}\ 2^{\alpha_2} \ldots k^{\alpha_k}|p]_1,$$

where the $b_{\underline{\alpha}}$ values are zero or positive constants varying with the particular partition of $\underline{\alpha} = (\alpha_1\ \alpha_2 \ldots \alpha_k)$.

Substituting s and n-s for u and using the equality relating the respective moment components, we may write

$$\left\{C_{\alpha}(s) - (-1)^{\alpha}C_{\alpha}(n-s)\right\}b_{\underline{\alpha}} + \left\{C_{\alpha 1}(s) - (-1)^{\alpha}C_{\alpha 1}(n-s)\right\}[1^{\alpha_1}\ 2^{\alpha_2} \ldots k^{\alpha_k}]_1$$
$$+ \left\{C_{\alpha 2}(s) - (-1)^{\alpha}C_{\alpha 2}(n-s)\right\}b_{\underline{\alpha}2}[1^{\alpha_1}\ 2^{\alpha_2} \ldots k^{\alpha_k} | 2]_1 + \ldots$$
$$\ldots + \left\{C_{\alpha p}(s) - (-1)^{\alpha}C_{\alpha p}(n-s)\right\}b_{\underline{\alpha}p}[1^{\alpha_1}\ 2^{\alpha_2} \ldots k^{\alpha_k}|p]_1 = 0.$$

Using the set of simultaneous equations which can be obtained by considering all moments of a given order it can easily be shown that only the trivial solution

$$C_{\alpha i}(s) - (-1)^{\alpha} C_{\alpha i}(n-s) = 0, \quad \text{for all } i$$

is possible, whence

$$C_{\alpha i}(s) = (-1)^{\alpha} C_{\alpha i}(n-s).$$

This result can also be verified by direct substitution.

4.0 RADIUS MULTIPLIERS AND ROTATABILITY

Having general formulas for the moment components contributed by each submatrix D_s of a derived design matrix D, we now seek a suitable set of radius multipliers such that the moments of D will fulfill the requirements for rotatability. Or, more specifically, such that the moments

$$[1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}] = \sum_{s=1}^{k} a_s^{\alpha} [1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}]_s$$

will be of the form listed under 3.1.

For convenience in describing these requirements we will refer to <u>even - order moments</u> as those for which $\alpha = \sum \alpha_i$ is even and <u>odd - - order moments</u> as those for which α is odd. In addition, let us define those moments for which <u>any</u> α_i is odd as <u>odd moments</u> and those where all α_i are even as <u>even moments</u>. Using these definitions, we can say that for rotatability all odd moments must equal zero and all even moments of the same order must be specified multiples of each other, <u>i.e</u>.,

$$[1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}] = \lambda_\alpha \frac{\prod_{i=1}^{k} (\alpha_i)!}{2^{\alpha/2} \prod_{i=1}^{k} (\frac{\alpha_i}{2})!}, \quad \text{all } \alpha_i \text{ even}$$

where λ_α is constant for a given design and α.

From Table 1 we see that the moments $[i]$, $[ij]$ and $[i^2]$ of D, will satisfy the rotatability requirements for any choice of radius multipliers since the corresponding odd moment components $[i]_s$ and $[i\ j]_s$ are identically zero and $[i^2]_s$ is constant for all i.

The other moments however all involve variable terms $C_{\alpha i}(s)\ [\quad]_1$ and only in the case of the even moments is the constant term $b_{\underline{\alpha}} C_\alpha(s)$

added to this variable function. It can be seen that 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 $[1^{\alpha_1}\ 2^{\alpha_2}\ \ldots\ k^{\alpha_k}]$. 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, $b_{\underline{\alpha}}C_{\alpha}(s)$, are in the required ratios.

In general then since

$$[1^{\alpha_1}\ 2^{\alpha_2}\ \ldots\ k^{\alpha_k}]_s = b_{\underline{\alpha}}C_{\alpha}(s) + C_{\alpha 1}(s)[1^{\alpha_1}\ 2^{\alpha_2}\ \ldots\ k^{\alpha_k}]_1$$

$$+ b_{\underline{\alpha 2}}C_{\alpha 2}(s)[1^{\alpha_1}\ 2^{\alpha_2}\ \ldots\ k^{\alpha_k}|2]_1 + \ldots + b_{\underline{\alpha p}}C_{\alpha p}(s)[1^{\alpha_1}\ 2^{\alpha_2}\ \ldots\ k^{\alpha_k}|p]_1,$$

where $b_{\underline{\alpha}}C_{\alpha}(s)$ does not appear unless the moment is even, we have

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

$$= b_{\underline{\alpha}}\sum_{s=1}^{k}(a_s)^{\alpha}C_{\alpha}(s) + [1^{\alpha_1}\ 2^{\alpha_2}\ \ldots\ k^{\alpha_k}]_1 \cdot \sum_{s=1}^{k}(a_s)^{\alpha}C_{\alpha 1}(s)$$

$$+ b_{\underline{\alpha 2}}[1^{\alpha_1}\ 2^{\alpha_2}\ \ldots\ k^{\alpha_k}|2]_1 \cdot \sum_{s=1}^{k}(a_s)^{\alpha}C_{\alpha 2}(s)$$

$$+ \ldots + b_{\underline{\alpha p}}[1^{\alpha_1}\ 2^{\alpha_2}\ \ldots\ k^{\alpha_k}|p]_1 \cdot \sum_{s=1}^{k}(a_s)^{\alpha}C_{\alpha p}(s),$$

where we require

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

Since we have shown 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, that when α and k are both odd, $C_{\alpha i}(\frac{n}{2}) = C_{\alpha i}(\frac{k+1}{2}) = 0$. 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 $m = \frac{k}{2}$ when k is even and $m = \frac{k-1}{2}$ when k is odd it then follows that

$$\sum_{s=1}^{k} (a_s)^{\alpha} C_{\alpha i}(s) = \sum_{s=1}^{m} (a_s)^{\alpha} [C_{\alpha i}(s) + C_{\alpha i}(n-s)]$$

$$= 0 \quad \text{for all } i, \ \alpha \text{ odd.}$$

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

$$[i^2] = \lambda_2$$
$$[i^2\ j^2] = \lambda_4$$
$$[i^4] = 3\lambda_4$$

where λ_2 and λ_4 are constant for any design. 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 will not change the general form of these moments since their only effect is to increase the denominator N. Hence if the moments of D satisfy the rotatability criterion we can add center points at will.

5.1 Application of Moment Requirements

As noted previously, 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.

We may generalize the expressions of Table 1 for fourth order moment components by letting the coefficient b_4 vanish for odd moments, such that, for $\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 = 4$

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

so that

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

In the previous section we showed that, for rotatability, we must have

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

making

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

Hence all odd moments of order four vanish with b_4 and

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

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

Any symmetric solution for the radius multipliers such that $\sum_{s=1}^{k} (a_s)^4 C_{41}(s) = 0$ will therefore clearly provide a rotatable design in that

(a) all odd order moments will be zero due to symmetry

(b) the odd fourth moments will equal zero

(c) $[i^2]$ will be the same for all i

(d) $[i^4]$ will equal $3[i^2 j^2]$, which will not depend on the choice of i and j

Such designs will be called simplex-sum designs.

5.2 Standard Solution for Radius Multipliers

The equation $\sum_{s=1}^{k} (a_s)^4 C_{41}(s) = 0$ was solved for the symmetric set of values $\{a_s\}$ in the specific cases of k = 2, 3, and 4. The results suggested that a <u>standard solution</u>, for any k, might be

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

which we shall henceforth denote by $B_s^{-\frac{1}{4}}$.

To prove the generality of this solution we substitute $B_s^{-\frac{1}{4}}$ in the general formula,

$$[1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}] = \sum_{s=1}^{k} \binom{n-2}{s-1}^{-\frac{\alpha}{4}} [1^{\alpha_1} 2^{\alpha_2} \ldots k^{\alpha_k}]_s$$

and show that a rotatable design results.

It is immediately evident that all odd moments will be zero since the set of values, $\left\{B_s^{-\frac{1}{4}}\right\}$, provide a symmetric solution as defined earlier. Further

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

Let u = s-1 and substitute k = n-1, then

$$[i^2] = \frac{n}{N} \sum_{u=0}^{n-2} \binom{n-2}{u}^{\frac{1}{2}} = \lambda_2$$

and, for each i, $[i^2]$ equals $\frac{n}{N}$ times the sum of the square roots of the binomial coefficients $\binom{n-2}{u}$.

$$[i\ j\ k\ l] = \sum_{s=1}^{n-1} \binom{n-2}{s-1}^{-\frac{4}{4}} \frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)} \binom{n-2}{s-1} [i\ j\ k\ l]_1$$

$$= \sum_{s=1}^{n-1} \frac{n^2 - 6sn + 6s^2 + n}{(n-2)(n-3)} [i\ j\ k\ l]_1$$

$$= \frac{[i\ j\ k\ l]_1}{(n-2)(n-3)} \left\{(n-1)n^2 - 6n[\tfrac{n}{2}(n-1)] + 6[\tfrac{n}{6}(n-1)(2n-1)] + (n-1)n\right\}$$

$$= \frac{[i\ j\ k\ l]_1}{(n-2)(n-3)} [0] = 0 .$$

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

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

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

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

$$= \frac{n^2}{N\ (n-2)(n-3)} \sum_{s=1}^{n-1} (s-1)(n-s-1)$$

$$= \frac{n^2(n-1)}{6N} = \lambda_4,$$

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

$$= \frac{n^2(n-1)}{2N} = 3\ \lambda_4.$$

We have thus demonstrated that sets of points satisfying the moment conditions of second order rotatable designs can be derived from those of first order. The solution $a_s = B_s^{-\frac{1}{4}}$ has been shown to apply for any number of variables greater than two ($k \geq 3$) since the fourth order moment formulas hold only for $n \geq 4$, as noted previously.

5.3 Second Order Rotatability for the Case n = 3

Using the formulas for fourth order moments for n = 3 in Table 1b, we can show in a similar way that $a_s = B_s^{-\frac{1}{4}} = \binom{n-2}{s-1}^{-\frac{1}{4}}$ also applies for k = 2.

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

$$= [i\ j^3]_1 - 5[i\ j^3]_1 .$$

This result, although apparently inconsistent with previous results in that $[i\ j^3]$ is not immediately zero via the route $\sum_{s=1}^{2} a_s^4\ C'_{41}(s) = 0$, will satisfy the moment requirements. The conditions are satisfied due to a property of 3 x 3 matrices of the type $[\underline{1}\ \underline{x}_1\ \underline{x}_2]$ with orthogonal columns that makes $[i\ j^3]_1 = 0$.

This property can be demonstrated algebraically, but since we have already shown that a matrix of all sums of rows taken s at a time is the negative of the matrix of sums taken n-s at a time we have $D_1 = -D_2$ and

$$[i\ j^3]_1 = [i\ j^3]_2 .$$

But the general moment formula for n = 3 shows

$$[i\ j^3]_2 = -5[i\ j^3]_1$$

Hence

$$[i\ j^3]_1 = -5[i\ j^3]_1$$

and must vanish.

Proceeding to the moment $[i^2\ j^2]$,

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

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

But since $[i^2\ j^2]_1 = [i^2\ j^2]_2$

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

or $$[i^2\ j^2]_1 = \frac{3}{2N},$$ a constant for any matrix of this type.

Hence $[i^2\ j^2] = 2[i^2 j^2]_1 = \frac{3}{N} = \lambda_4$.

Similarly the moment $[i^4]$ is found to be

$$[i^4] = 3\ \lambda_4$$

and therefore the moments are those of a rotatable design. This result agrees with that obtained in (12) and shows that it is a special case of the standard solution $a_s = B_s^{-\frac{1}{4}}$.

While these designs satisfy the moment requirements for rotatability, they yield a singular, or almost singular, moment matrix. Thus to become usable designs they require the addition of center points (to be discussed in Section 7.3).

6.0 THIRD ORDER REQUIREMENTS FOR ROTATABILITY

To prove that the derived matrix D possesses the moments required for third order rotatability it is necessary to show that a set of radius multipliers can be found which will not only satisfy the requirements for second order rotatability, but will also

(a) make all fifth order moments equal to zero,

(b) make all terms in the sixth order moments involving moment components of D_1 other than $[i^2]_1$ sum to zero.

A symmetric solution will again satisfy the requirements of (a) above. From Table 1 we see that part (b) can be accomplished if we find a_s such that

$$\sum_{s=1}^{k} (a_s)^6 \, C_{6i}(s) = 0$$

where i = 1, 2, 3.

This result will hold true for all sixth order moments and therefore we need only find a symmetric solution for this set of three simultaneous equations involving a_s^6 which will also satisfy the corresponding fourth order moment equation involving a_s^4.

To do this we will solve the sixth order set of three equations and see if a feasible solution is obtained. If we let $a_s^6 = a_{s6}$ we may consider them as a set of homogeneous linear equations for each value of n,

$$A\underline{a}_6 = 0$$

where

$$\underline{a}_6 = (a_{16} \; a_{26} \; \cdots \; a_{k6})'$$

and

$$A = \begin{bmatrix} C_{61}(1) & C_{61}(2) & \cdots\cdots & C_{61}(k) \\ C_{62}(1) & C_{62}(2) & \cdots\cdots & C_{62}(k) \\ C_{63}(1) & C_{63}(2) & \cdots\cdots & C_{63}(k) \end{bmatrix} .$$

As our moment equations do not hold for $n \leq 5$ we will begin with the minimum value of $n = 6$.

Substituting in $C_{6i}(s)$ we have

$$A = \begin{bmatrix} 1 & -26 & 66 & -26 & 1 \\ 0 & 1 & -4 & 1 & 0 \\ 0 & 1 & -2 & 1 & 0 \end{bmatrix} .$$

However this matrix is equivalent by row operations to a matrix

$$A^* = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} .$$

Hence the solution for $A\underline{a}_6 = 0$ demands that

$$a_{16} = -a_{66},$$
$$a_{26} = -a_{56},$$
$$a_{36} = 0,$$

which is not a feasible solution since all $a_{i6} = a_i^6$ must be positive for real radius multipliers. We have thus shown the design matrix D for $n = 6$ is not third order rotatable.

Similarly we find that for the case n = 7

$$A = \begin{bmatrix} 1 & -25 & 40 & 40 & -25 & 1 \\ 0 & 1 & -3 & -3 & 1 & 0 \\ 0 & 1 & -1 & -1 & 1 & 0 \end{bmatrix},$$

and

$$A^* = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

for which no feasible solution can be obtained.

For n = 8

$$A = \begin{bmatrix} 1 & -24 & 15 & 80 & 15 & -24 & 1 \\ 0 & 1 & -2 & 6 & -2 & 1 & 0 \\ 0 & 1 & 0 & -2 & 0 & 1 & 0 \end{bmatrix}$$

and

$$A^* = \begin{bmatrix} 1 & 0 & 0 & 92 & 0 & 0 & 1 \\ 0 & 1 & 0 & -2 & 0 & 1 & 0 \\ 0 & 0 & 1 & -4 & 1 & 0 & 0 \end{bmatrix}.$$

For n = 9

$$A = \begin{bmatrix} 1 & -23 & -9 & 95 & 95 & -9 & -23 & 1 \\ 0 & 15 & -15 & -120 & -120 & -15 & 15 & 0 \\ 0 & 10 & 10 & -20 & -20 & 10 & 10 & 0 \end{bmatrix}.$$

and

$$A^* = \begin{bmatrix} 1 & 0 & 0 & 7 & 7 & 0 & 0 & 1 \\ 1 & 1 & 0 & -5 & -5 & 0 & 1 & 0 \\ 0 & 0 & 1 & 3 & 3 & 1 & 0 & 0 \end{bmatrix}.$$

Neither of these matrices yield solutions such that all $a_{16} \geq 0$.

Since a polynomial of degree three has $\binom{k+3}{3}$ constants, a third order design must have at least this many points. Therefore k must be at least five before D has sufficient experimental points to be considered a candidate. We have thus demonstrated that D cannot be third order rotatable for $k \leq 8$. It would appear impractical to consider designs involving more than 8 variables. The size of the experiment alone approaches prohibitive proportions as a minimum of 220 experimental points is required for $k = 9$.

7.0 SECOND ORDER ROTATABLE SIMPLEX-SUM DESIGNS: THE STANDARD SOLUTION

We have shown previously, in Section 5.2, that the derived design matrix D can be made second order rotatable by using a set of radius multipliers $a_s = \binom{n-2}{s-1}^{-\frac{1}{4}}$. Before proceeding to show that other specific solutions are possible in higher dimensionality, we will first investigate the effect that the choice of radius multipliers has on the geometric configuration of the design in the factor space.

It was noted earlier that the points in k space described by any n by k first order rotatable design matrix, D_1, are the vertices of a regular simplex. When we add those vectors two at a time the vector which is generated will pass through the midpoint of the edge of the simplex connecting these two points. Sums of three vectors have a resultant passing through the midpoints of the faces. While sums taken s at a time for $s > 3$ cannot be visualized in as few dimensions, some concept of the geometry of the design can be obtained through the extension of this idea of the average or midpoint vector of s symmetrically spaced vectors. To complete the feeling for these designs we must find the relative distances along these vector directions to the specified design points.

7.1 Radius of Experimental Points

The radius of an experimental point is its distance in the factor space from the geometric center of the design, which we took as the origin of coordinates. Considering the coordinates of the point as a vector, the radius is the length of that vector. To obtain a general expression for the length of the row vectors in each submatrix D_s we may denote its u^{th} row as $\underline{x}'_{su}$, $s = 2, 3, \ldots, k$. Then

$$\underline{x}'_{su} = \underline{x}'_{u_1} + \underline{x}'_{u_2} + \ldots \underline{x}'_{u_s}$$

where $\underline{x}'_{u_1}, \underline{x}'_{u_2}, \ldots, \underline{x}'_{u_s}$ is the u-th set of s rows of the first order design matrix D_1. Now since

$$[\underline{1}\ D_1] = \begin{bmatrix} 1 & \underline{x}'_1 \\ 1 & \underline{x}'_2 \\ \vdots & \\ 1 & \underline{x}'_k \end{bmatrix}$$

and $[\underline{1}\ D_1]'\ [\underline{1}\ D_1] = n\ I_n$ we have

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

The square of the length of the row vector $\underline{x}'_{su}$ can be written

$$\begin{aligned} L_s^2 &= \underline{x}'_{su}(\underline{x}'_{su})' = \underline{x}'_{su}\ \underline{x}_{su} \\ &= (\underline{x}'_1 + \underline{x}'_2 + \ldots + \underline{x}'_s)(\underline{x}_1 + \underline{x}_2 + \ldots + \underline{x}_s) \\ &= s(n-1) + 2\binom{s}{2}(-1) \\ &= s(n-s). \end{aligned}$$

Thus the radius of the experimental points in the submatrix $a_s D_s$ of the design matrix D must follow as

$$r_s^2 = (a_s L_s)^2 = a_s^2\ s(n-s)$$

$$r_s = a_s\ [s(n-s)]^{\frac{1}{2}}.$$

It is evident that $r_s = r_{n-s}$ since the points are reflections of each other through the origin.

7.2 Radii for the Standard Solution

For the particular set of radius multipliers of the standard solution, i.e., $a_s = \binom{n-2}{s-1}^{-\frac{1}{4}}$, the radii will be

$$r_s = \binom{n-2}{s-1}^{-\frac{1}{4}} [s(n-s)]^{\frac{1}{2}}.$$

A summary of the radii for k = 2 through 8 of the standard solution rotatable designs follows in Table 2.

Table 2. Radii of experimental points for standard solution rotatable designs

k	r_1	r_2	r_s	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

7.3 Singularity and Near Singularity of Moment Matrices

It is shown in (12) that a set of points can have the moments of a rotatable design of order 2 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 X matrix for the b_0 and quadratic terms, $b_{11}, b_{22}, \ldots, b_{kk}$. The situation is easily remedied, however, by the addition of center points to the design matrix, so that the appearance of this property need not concern us too much.

As shown in (12) the moment matrix will be singular when the standardized fourth moment constant λ_4' achieves the value

$$\lambda_4' = \frac{\lambda_4}{(\lambda_2)^2} = \frac{k}{k+2},$$

implying that the design points all lie on the same hypersphere (4). For the designs arising from the standard solution for a_s we have

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

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

where we have used $N = 2^n - 2$.

The value for λ_4' is equal to the singular value $\left(\frac{k}{k+2}\right)$ when $k = 2$ and remains close to the singular value as k increases, as is shown in Table 3.

Table 3. Comparison of λ_4' to its singular value

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

Since the addition of center points has no effect on the moments except to change N we see that the addition of N_o center points will change λ_4' by a factor of $\frac{2^n - 2 + N_o}{2^n - 2}$. The addition of center points serves other useful purposes however. First it provides an estimate of error for testing the adequacy of the model and secondly it affects the shape of the variance function (12). As is true for other designs (e.g., factorials) which might be used in response surface experimentation, the variance of an estimated response is usually relatively high at the center of the design, decreases to a minimum and then rises rapidly as $\rho = \sqrt{\underline{x}' \underline{x}}$ approaches the radii of the outer design points. By adding the proper number of center points the variance at the center can be reduced so that the variance is more or less uniform over what is usually the principal region of interest. If the number of center points required to attain this is not economical a compromise can be reached. In general it is suggested in (12) that uniform variance can be approximated for rotatable designs by adding sufficient points at the center to equate the variance at $\rho = 0$ to that at $\rho = 1$ in terms of standardized units (i.e., x_i scaled so that $\sum_u x_{iu}^2 = N$). For the unstandardized units usually used in actual designs this implies equating the variance at $\rho = 0$ to that at $\rho = \sqrt{\lambda_2}$.

8.0 ADDITIONAL SECOND ORDER ROTATABLE SIMPLEX-SUM DESIGNS

The standard solution for a_s affords a set of rotatable designs for all $k \geq 2$. When $k \geq 5$ however, we shall demonstrate that other specific solutions for the radius multipliers are possible. Further, since the number of experiments required by the standard solution soon becomes excessive we shall seek sets of radius multipliers which include some zeros thereby providing smaller, reduced designs.

8.1 Solution Space of Radius Multipliers

We have shown in Section 5 that for second order rotatability we must find values for a_s, $s = 1, 2, \ldots, k$, 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 D_1 (Table 1). 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 vectors of linear components

$$\underline{a} = (a_1 \; a_2 \ldots a_s \ldots a_k)'$$

$$\underline{a}_3 = (a_1^3 \; a_2^3 \ldots a_s^3 \ldots a_k^3)' = (a_{13} \; a_{23} \ldots a_{s3} \ldots a_{k3})',$$

and

$$\underline{a}_4 = (a_1^4 \; a_2^4 \ldots a_s^4 \ldots a_k^4)' = (a_{14} \; a_{24} \ldots a_{s4} \ldots a_{k4})'.$$

Let us also define row vectors

$$\underline{C}_{31}' = (C_{31}(1) \; C_{31}(2) \ldots\ldots C_{31}(s) \ldots\ldots C_{31}(k)),$$

$$\underline{C}_{41}' = (C_{41}(1) \; C_{41}(2) \ldots\ldots C_{41}(s) \ldots\ldots C_{41}(k)),$$

whose elements are the moment component coefficients.

We may therefore restate the requirements for second order rotatability in our present situation as that of finding a set of radius multipliers such that $\underline{C}_{31}'\underline{a}_3 = 0$ and $\underline{C}_{41}'\underline{a}_4 = 0$. But if we choose symmetric values of $\underline{a}_s$, such that $a_s = a_{n-s}$, we have shown previously that $\underline{C}_{31}'\underline{a}_3 = 0$. Therefore, calling any vectors $\underline{a}_3$ and $\underline{a}_4$ which are derived from symmetric solutions, <u>symmetric vectors</u>, we may further simplify our problem to that of finding all symmetric vectors $\underline{a}_4$ such that $\underline{C}_{41}'\underline{a}_4 = 0$. We must also add the restriction of course, that $\underline{a}_4 \geq \underline{0}$.

The restriction of symmetry on the vector $\underline{a}_4$ has the effect of confining its values to an m dimensional subspace where

$$m = \frac{k}{2}, \text{ if } k \text{ even}$$

and

$$m = \frac{k+1}{2}, \text{ if } k \text{ is odd.}$$

This is evident since $\underline{a}_4$ 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 $\underline{C}_{41}$ are symmetric in a corresponding way as was shown earlier. Hence for convenience we might consider $\underline{a}_4$ and $\underline{C}_{41}$ 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 $\underline{C}_{41}'\underline{a}_4 = 0$ they will form a basis for the solution space of all possible vectors satisfying the equation, (<u>i.e.</u>, all vectors in the m-1 space orthogonal to $\underline{C}_{41}$). Since the elements of $\underline{C}_{41}$ are of mixed sign it is clear that solution vectors can be found which fall in the positive 2^k -drant.

8.2 Specific Solutions

We will now obtain the m-1 basis vectors $\gamma_1, \gamma_2, \dots \gamma_{m-1}$ for $k = 3, 4, \dots 8$, 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, corresponding to points at the origin, may be eliminated from D without altering the moments. All other designs, resulting from the orthogonality relationship, can be derived from these basis vectors by taking linear combinations

$$\underline{a}_4 = d_1\gamma_1 + d_2\gamma_2 + \dots + d_{m-1}\gamma_{m-1},$$

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

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 $k = 2$, $\underline{C}'_{41}\underline{a}_4 \neq 0$ 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, $(\gamma_1 = \underline{a}_4)$.

Therefore

$$\underline{C}'_{41}\underline{a}_4 = (1 \quad -4 \quad 1) \begin{bmatrix} 1 \\ \frac{1}{2} \\ 1 \end{bmatrix} = 0,$$

$$\underline{a} = (1 \quad 2^{-\frac{1}{4}} \quad 1)' = \underline{B}_s^{-\frac{1}{4}},$$

where the k elements of the vector $\underline{B}_s^{-\frac{1}{4}}$ are the $B_s^{-\frac{1}{4}}$ values of the standard solution.

The one modification of the design possible, of course, is multiplication by a constant ($\underline{i.e.}$, $\underline{a}_4 = d_1\gamma_1$) which merely amounts to a scaling change.

When k = 4, again m = 2 and the standard solution is again unique

$$\underline{C}'_{41}\underline{a}_4 = (1 \quad -3 \quad -3 \quad 1) \begin{bmatrix} 1 \\ \frac{1}{3} \\ \frac{1}{3} \\ 1 \end{bmatrix} = 0$$

and

$$\underline{a} = (1 \quad 3^{-\frac{1}{4}} \quad 3^{-\frac{1}{4}} \quad 1)' = \underline{B}_s^{-\frac{1}{4}}.$$

When k = 5 m = 3 and two independent solutions γ_1 and γ_2 are possible.

$$\underline{C}'_{41}\,\gamma_i = (1 \quad -2 \quad -6 \quad -2 \quad 1)\gamma_i = 0.$$

Here, for the first time, we can obtain reduced designs. Both basis vectors will be of this type where

$$\gamma_1 = (1 \quad 0 \quad \tfrac{1}{3} \quad 0 \quad 1)'$$

$$\gamma_2 = (1 \quad \tfrac{1}{2} \quad 0 \quad \tfrac{1}{2} \quad 1)'$$

and

$$\underline{a} = (1 \quad 0 \quad 3^{-\frac{1}{4}} \quad 0 \quad 1)',$$

$$\underline{a} = (1 \quad 2^{-\frac{1}{4}} \quad 0 \quad 2^{-\frac{1}{4}} \quad 1)'.$$

The design resulting from γ_1 omits D_2 and D_4 while the γ_2 design omits D_3 from the design.

To demonstrate that the standard solution is spanned by these vectors

$$\underline{a}_4 = \frac{1}{2}\gamma_1 + \frac{1}{2}\gamma_2 = (1 \quad \frac{1}{4} \quad \frac{1}{6} \quad \frac{1}{4} \quad 1)'$$

from which the standard solution is obtained,

$$\underline{a} = (1 \quad 4^{-\frac{1}{4}} \quad 6^{-\frac{1}{4}} \quad 4^{-\frac{1}{4}} \quad 1)' = \underline{B}_s^{-\frac{1}{4}}.$$

Any other linear combination such that $\underline{a}_4 \geq 0$ would also provide a solution as for example

$$\underline{a}_4 = \frac{3}{5}\gamma_1 + \frac{2}{5}\gamma_2 = (1 \quad \frac{1}{5} \quad \frac{1}{5} \quad \frac{1}{5} \quad 1)',$$

and

$$\underline{a} = (1 \quad 5^{-\frac{1}{4}} \quad 5^{-\frac{1}{4}} \quad 5^{-\frac{1}{4}} \quad 1)'.$$

When k = 6, m = 3 resulting in two independent reduced solutions,

$$\underline{C}'_{41}\gamma_i = (1 \quad -1 \quad -8 \quad -8 \quad -1 \quad 1)\gamma_i = 0,$$

$$\gamma_1 = (1 \quad 1 \quad 0 \quad 0 \quad 1 \quad 1)',$$

$$\gamma_2 = (1 \quad 0 \quad \frac{1}{8} \quad \frac{1}{8} \quad 0 \quad 1)'$$

and the specific solution can be obtained by taking the fourth root of each element.

When k = 7, m = 4 and three independent vectors of radius multipliers can be found

$$\underline{C}'_{41}\gamma_i = (1 \quad 0 \quad -9 \quad -16 \quad -9 \quad 0 \quad 1)\gamma_i = 0$$

$$\gamma_1 = (1 \quad 0 \quad \frac{1}{9} \quad 0 \quad \frac{1}{9} \quad 0 \quad 1)'$$

$$\gamma_2 = (1 \quad 0 \quad 0 \quad \frac{1}{8} \quad 0 \quad 0 \quad 1)'$$

$$\gamma_3 = (0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0)'.$$

When $k = 8$, $m = 4$ providing three basis vectors

$$\underline{c}_{41}'\gamma_1 = (1 \quad 1 \quad -9 \quad -25 \quad -25 \quad -9 \quad 1 \quad 1)\ \gamma_1 = 0,$$

$$\gamma_1 = (1 \quad 0 \quad \tfrac{1}{9} \quad 0 \quad 0 \quad \tfrac{1}{9} \quad 0 \quad 1)',$$

$$\gamma_2 = (1 \quad 0 \quad 0 \quad \tfrac{1}{25} \quad \tfrac{1}{25} \quad 0 \quad 0 \quad 1)',$$

$$\gamma_3 = (0 \quad 1 \quad \tfrac{1}{9} \quad 0 \quad 0 \quad \tfrac{1}{9} \quad 1 \quad 0)'.$$

A fourth reduced design can be derived from the following vector

$$\underline{a}_4 = \gamma_2 - \gamma_1 + \gamma_3 = [0 \quad 1 \quad 0 \quad \tfrac{1}{25} \quad \tfrac{1}{25} \quad 0 \quad 1 \quad 0]'.$$

A summary of the radius multipliers used to obtain the standard solution designs ($B_s^{-\frac{1}{4}}$) 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" within a hypersphere of radius $\sqrt{\lambda_2}$.

In order to produce a design using Table 4, it is only necessary to select a suitable matrix 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 D_s matrices. Multiplication of D_s by a_s will then give the coordinates of the design points. An example is given in Section 11.

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		
	γ_2	1	.8409	0	.8409	1				42	10		
	γ_1	1	0	.7598	0	1				32	8	26	6
6	Std.	1	.6687	.5623	.5623	.6687	1			126	38		
	γ_2	1	0	.5946	.5946	0	1			84	16		
	γ_1	1	1	0	0	1	1			56	13	44	9
7	Std.	1	.6389	.5081	.4729	.5081	.6389	1		254	59		
	γ_1	1	0	.5774	0	.5774	0	1		128	21		
	γ_2	1	0	0	.5946	0	0	1		86	15		
	γ_3	0	1	0	0	0	1	0		56	10	78	14
8	Std.	1	.6150	.4671	.4111	.4111	.4671	.6150	1	510	90		
	γ_2	1	0	0	.4472	.4472	0	0	1	270	26		
	γ_3	0	1	.5774	0	0	.5774	1	0	240	0		
	γ_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 (12) 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 $\rho = \sqrt{\lambda_2}$.

9.0 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., D_s and D_{n-s} are replicated equally), thus ensuring that a symmetric solution for the radius multipliers can be found.

If we replicate a particular set of submatrices D_s and 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

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

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 $\nu_1 a_1{}^4 = 1$, $\nu_2 a_2{}^4 = 1/2$, $\nu_3 a_3{}^4 = 1$.) 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	$2^{-1/4}$	1	1.73	1.68	1.73
2	2	1	2	$2^{-1/4}$	$2^{-1/4}$	$2^{-1/4}$	1.45	1.68	1.45
3	1	8	1	1	2^{-1}	1	1.73	1.00	1.73

10.0 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 (12) then we will assume the expected value of the u^{th} experimental observation is represented by the model

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

where β_{ow} is the level parameter for the w^{th} block and z_{wu} is a dummy variable assuming the value unity when the u^{th} experiment falls in block w and zero otherwise.

We might arbitrarily define β_o as the weighted average of the β_{ow}'s so that the model above can be rewritten in an equivalent form but which is now identical to the model when no blocking is used except for the addition of an incremental block effect. That is

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

where

$$\beta_o = \sum_{w=1}^{m} \frac{n_w}{N} \beta_{ow} , \quad \delta_w = \beta_{ow} - \beta_o , \quad \bar{z}_w = \frac{n_w}{N}$$

and n_w is the number of observations in the w^{th} block (including centerpoints) and $N = \sum_{w=1}^{m} n_w$.

10.1 Orthogonal Blocking - Rotatable Designs

It is shown in (12) 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. $[i]_{bw} = \frac{1}{N} \sum_{u}^{n_w} x_{iu} = 0$, $w = 1, 2 \ldots m$

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

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

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

Orthogonal blocking ensures that, in the normal equations, the portion involving the regression coefficients will be free of block effects and hence the estimation of the vector of regression coefficients (b̲) proceeds as though there were no blocking. General formulas for estimating the elements of b̲ are given in (12) together with expressions for their variances. The only departure from the analysis of an unblocked experiment is the removal of the block sum of squares from the residual sum of squares in estimating the error.

Simplex-sum designs lend themselves to orthogonal blocking in most cases although not always in manageable block sizes as we shall see.

From the general formulas for the moment components of the submatrices D_1, D_2, ... D_k we see that conditions 1 and 2 for orthogonal blocking will automatically be satisfied if we use these partitions, or combinations of these partitions, of the design matrix as blocks. For convenience we shall refer to blocking schemes of this sort as <u>sub-matrix blocking schemes</u>. Submatrix blocking is desirable in that each D_s is a first order rotatable design and hence provides an easily identified natural set of blocks for sequential experimentation. Unfortunately, however, these submatrices do not in general satisfy the third condition for orthogonal blocking, although as will be shown later, they come quite close.

For a standard solution design the block second-moment component of D_s is

$$[i^2]_{bs} = a_s^2\,[i^2]_s = \binom{n-2}{s-1}^{1/2} \frac{n}{N}\,.$$

Now to satisfy condition 3 for orthogonal blocking we would require

$$\frac{[i^2]_{bs}}{\lambda_2} = \frac{\binom{n-2}{s-1}^{1/2}}{\sum_{s=1}^{k} \binom{n-2}{s-1}^{1/2}} \quad \text{to equal} \quad \frac{n_s}{N} = \frac{\binom{n}{s} + n_{so}}{2^n - 2 + N_o}$$

where n_{so} denotes the number of center points added to block s, (<u>i.e.</u>, D_s), and $N_o = \sum n_{so}$. Since the ratio $[i^2]_{bs} / \lambda_2$ will in general involve the ratio of irrational numbers, it is clear that exact orthogonality cannot usually be obtained by considering the <u>individual</u> submatrices as blocks. The one exception is the two factor hexagon design where, since n = 3, the binomial coefficients are 1 and hence rational numbers are obtained. This proves the simplest case, however, of a general orthogonal blocking scheme since whenever k is even, two orthogonal blocks are easily formed by combining $D_1, D_2 \cdots D_{k/2}$ in one block and the remaining half of D in the second block. Then since

$$a_s^2\,[i^2]_s = a_{n-s}^2\,[i^2]_{n-s}$$

$$[i^2]_{bw} = \sum_{s=1}^{k/2} a_s^2\,[i^2]_s \qquad w = 1, 2$$

$$\frac{[i]_{bw}}{\lambda_2} = \frac{n_w}{N} = \frac{1}{2}$$

as long as an equal number of center points (if any) is added to each block. However, since $n_w = 2^k - 1 + n_{wo}$ the block size grows quite rapidly and for many situations may be excessive. When k is odd no such simple orthogonal blocking exists since splitting $D_{(k+1)/2}$ into symmetric halves results in losing the property $[i]_{bw} = 0$.

This same general scheme can be used for specific solution designs and here, even when k is odd, we can form two orthogonal blocks as long as $k \geq 5$ since in all cases reduced designs exist in which $a_{(k+1)/2} = 0$ (Table 4). Thus, with the exception of the k = 3 case, simplex-sum designs are always available which can be divided into two orthogonal blocks and only in the five factor design are we forced to use other than the design requiring the fewest number of points to obtain orthogonality.

A few other designs which block orthogonally exist among the specific solutions. In these designs the individual submatrices may be used as blocks, but center points must be added in a specified manner. For specific solution designs condition 3 can be satisfied whenever the non-zero a_s^2 are rational. Referring to Section 8.2 it can be seen that among the designs listed such solution vectors of radius multipliers exist for k = 6 (γ_1), k = 7 (γ_1, γ_3) and k = 8 (γ_1, γ_2, γ_3). For these designs values of n_{so} have been found which satisfy 3 and also satisfy or approximate the conditions for "uniform variance" within a sphere of radius $\sqrt{\lambda_2}$. These blocking schemes are summarized in Table 6.

Table 6. Summary of orthogonal blocking schemes for rotatable designs of Table 4

k	Design	Block	Number of Points in Block from Submatrix								Total Number 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	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	γ_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
	γ_2	1	7		35						42	8	50
		2				35		7			42	8	50
	γ_1	1	7	21							28	6	34
		2					21	7			28	6	34
	γ_1	1	7								7	(0)	7
		2		21							21	(14)	35
		3					21				21	(14)	35
		4						7			7	(0)	7
7	γ_1	1	8		56						64	10	74
		2					56		8		64	10	74
	γ_3	1		28							28	5	33
		2						28			28	5	33
	γ_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
	γ_2	1	9			126					135	13	148
		2					126			9	135	13	148
	γ_3	1		36	84						120	0	120
		2						84	36		120	0	120
	γ_1	1	9		84						93	14	107
		2						84		9	93	14	107
	γ_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
	γ_3	1		36							36	(48)	84
		2			84						84	(0)	84
		3						84			84	(0)	84
		4							36		36	(48)	84
	γ_1	1	9								9	(4)	13
		2			84						84	(7)	91
		3						84			84	(7)	91
		4								9	9	(4)	13

The entries in the body of the table represent the number of experimental points contributed to the block by the particular column heading in which they fall. Except for those values in brackets the listed center points are those required for approximately "uniform variance" and could be replaced by any number as long as they were evenly distributed among blocks. Those values in brackets, however, are the numbers closest to those giving uniform variance which will give orthogonal blocking. They cannot be altered without checking for loss of orthogonality.

10.2 Orthogonal Blocking - Nearly Rotatable Designs

Orthogonal submatrix blocking can always be obtained by adjusting the radius multipliers and sacrificing rotatability. Since it will prove that very small adjustments are required, and hence small departures from rotatability are to be expected, this approach has much to recommend it. However, there is also a major drawback to changing the a_s values for the very general designs being considered here. If the radius multipliers are adjusted so that they remain symmetric, the odd third moments will vanish as for rotatable designs; the odd fourth order moments will not, however. Further, as will be recalled from Table 1, all fourth order moments may vary depending upon the choice of i, j, k, ℓ. Hence, the solution of the normal equations will in general involve the inversion of a matrix having $(k^2 + k + 2)/2$ elements on a side and not having sufficient pattern to allow a general inverse to be found. In special cases, of course, this does not occur (as for the central composite design of k = 3 where $[i\ j\ k\ \ell]_1$, $[i\ j\ k^2]_1$, and $[i\ j^3]_1$ are all zero). However, since we are dealing with completely general simplex-sum designs here, this approach is not too appealing, in that it requires considerable computation.

In the interests of completeness, however, and in view of the widespread availability of high speed computing machines, the radius multipliers required for orthogonal submatrix blocking of the Table 4 designs are tabulated in Table 7. These values are based on the number of center points required for uniform variance and will, of course, vary if the number of center points is changed. Those designs for which orthogonal rotatable blocking is available are omitted.

Comparison of these radius multipliers with those of Table 4 will show that the adjustment has been very small and indicates how surprisingly closely the submatrices approach the conditions for orthogonal blocking. In raising these to the fourth power however the difference becomes more sizeable and is quite effective in causing the unwanted components of the fourth order moments to be retained.

10.3 Non-Orthogonal Blocking of the Rotatable Designs

A third approach to submatrix blocking is to accept the small loss in efficiency suffered through using these slightly non-orthogonal sets as blocks. The estimates of the regression coefficients will then be the solution of more complicated normal equations but ones for which the general form of the solution is readily found as in the orthogonal case. The question then arises, under what conditions will the variance contours of an estimated response remain rotatable when the b's are solutions of the adjusted normal equations.

While the loss of rotatability would be unimportant here, since the departure would be small, the question is of general interest and worth

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						
	γ_2	1	1	.8238	4	0	0	.8238	4	1	1						
	γ_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				
	γ_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		
	γ_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

a short digression to develop the general conditions under which rotatability is retained. The development that follows will then be useful in obtaining the general solution for the regression coefficients and their variances.

10.3.1 Restrictions on Non-Orthogonal Blocking Necessary to Retain Rotatability. Expressing the general model, adopted at the start of Section 10, in matrix notation we have after ordering the trials by blocks

$$\underline{\eta} = X\underline{\beta} + Z^*\underline{\delta}^*$$

where

$\underline{\eta}$ is an N x 1 matrix of expected values ,

X is an N x (k + 1)(k + 2)/2 matrix of independent variables and is of full rank,

$\underline{\beta} = (\beta_0 \mid \beta_1^2\ \beta_2^2 \cdots \beta_k^2 \mid \beta_1\ \beta_2 \cdots \beta_k \mid \beta_{12}\ \beta_{13} \cdots \beta_{k-1,k})'$,

Z^* is an N x m matrix whose column vectors $\underline{z}_w$ are independent of the column vectors of X and are defined as

$$\underline{z}_w = \frac{1}{N} \begin{bmatrix} -n_w\, \underline{1}_{n_1} \\ \hdashline -n_w\, \underline{1}_{n_2} \\ \hdashline \vdots \\ \hdashline (N - n_w)\, \underline{1}_{n_w} \\ \hdashline \vdots \\ \hdashline -n_w\, \underline{1}_{n_m} \end{bmatrix},$$

$\underline{1}_{n_w}$ is an n_w x 1 column vector of unit elements

and $\underline{\delta}^*$ is an m x 1 column vector of the incremental block effects.

The columns of Z^* are dependent since $Z^* \underline{1}_m = \underline{0}$ but it is readily shown that any m - 1 of them are independent. If we drop one column from Z^* ($\underline{z}_m$ say) the remaining column vectors will be a basis for the same space and hence this will have no effect on the estimates of $\underline{\beta}$. We will denote this N x (m - 1) matrix by Z. This is equivalent to letting $\delta_m = 0$ in the model and hence the $\underline{\delta}^*$ vector is replaced by an (m - 1) x 1 vector $\underline{\delta}$ whose elements will be different but we are not usually interested in estimating these parameters in any event. Thus we may rewrite the model, now of full rank, as

$$\underline{\eta} = X\underline{\beta} + Z\underline{\delta} ,$$

and the normal equations become

$$X'X\underline{b} + X'Z\underline{d} = X'\underline{y}$$

$$Z'X\underline{b} + Z'Z\underline{d} = Z'\underline{y} ,$$

where $\underline{y}$ is an N x 1 vector of observations and $\underline{b}$ and $\underline{d}$ are the least squares estimates of $\underline{\beta}$ and $\underline{\delta}$ respectively. Eliminating $\underline{d}$ from the least squares equations for $\underline{b}$ we get the usual adjusted normal equations

$$[X'X - X'Z\,[Z'Z]^{-1}\,Z'X]\,\underline{b} = [X' - X'Z\,[Z'Z]^{-1}\,Z']\,\underline{y} ,$$

or letting $\dot{X}' = [X' - X'Z\,[Z'Z]^{-1}\,Z']$ for simplicity

$$\dot{X}'\dot{X}\underline{b} = \dot{X}'\underline{y} .$$

Under our assumptions of full rank above, $\dot{X}'\dot{X}$ must be non-singular and we have $V(\underline{b}) = [\dot{X}'\dot{X}]^{-1}\,\sigma^2$. It may now be determined under what blocking conditions $[\dot{X}'\dot{X}]^{-1}$ will be of the form required to retain rotatability given that our original design was rotatable.

It will be convenient to utilize Schlaflian matrices and power vectors here (1, 2, 30) in a manner similar to that developed in (12). Letting $\underline{x}' = [1\ x_1\ x_2\ \ldots\ x_k]$ we denote the derived second degree power vector by $\underline{x}'^{[2]}$ defined such that $\underline{x}'^{[2]}\underline{x}^{[2]} = [\underline{x}'\underline{x}]^2$. We will also require the second Schlaflian matrix $H^{[2]}$ which is defined such that if $\underline{z} = H\underline{x}$ then $\underline{z}^{[2]} = H^{[2]}\underline{x}^{[2]}$.

In terms of these matrices then the marginal model, ignoring block effects (except for our definition of β_o), may be written

$$\eta_u = \underline{x}_u'^{[2]} \underline{\beta}_s$$

where the elements of $\underline{\beta}_s$ are the same as those in $\underline{\beta}$ except that the linear and interaction terms are divided by $\sqrt{2}$ to compensate for the corresponding coefficients in

$$\underline{x}_u'^{[2]} = [1, | x_1^2, x_2^2, \dots x_k^2 \,|\, \sqrt{2}\,x_1, \sqrt{2}\,x_2, \dots \sqrt{2}\,x_k \,|\, \sqrt{2}\,x_1x_2 \dots].$$

In general we will use the subscript s to denote matrices adjusted for power vector constants. We will denote the moment matrix arising from the use of power vectors then by $X_s'X_s$, i.e.,

$$X_s'X_s = \sum_{u=1}^{N} \underline{x}_u^{[2]} \underline{x}_u'^{[2]}.$$

Now for $V(\hat{y}) = V(\underline{x}'^{[2]} \underline{b}_s)$ to be a function of $\underline{x}'\underline{x} = \rho^2$ alone

$$V(\hat{y}) = \underline{x}'^{[2]} [\dot{X}_s' \dot{X}_s]^{-1} \underline{x}^{[2]} \sigma^2$$

must be invariant under rotation. Hence, if $\underline{z} = R\underline{x}$, where

$$R = \left[\begin{array}{c|c} 1 & \underline{0}_k' \\ \hline \underline{0}_k & H \end{array}\right]_{(k+1) \text{ by } (k+1)},$$

H is orthogonal and $\underline{0}_k$ denotes a k by 1 vector of zeros, then

$$\underline{x}'^{[2]} [\dot{X}_s'\dot{X}_s]^{-1} \underline{x}^{[2]} = \underline{x}'^{[2]} R'^{[2]} [\dot{X}_s'\dot{X}_s]^{-1} R^{[2]}\underline{x}^{[2]}$$

and since this must hold for all $\underline{x}^{[2]}$ we may take advantage of the uniqueness of the inverse of a matrix and write

$$\dot{X}_s'\dot{X}_s = R'^{[2]} \dot{X}_s'\dot{X}_s R^{[2]}.$$

Hence

$$X_s'X_s - X_s' Z[Z'Z]^{-1} Z'X_s = R'^{[2]} X_s'X_sR^{[2]} - R'^{[2]} X_s'Z[Z'Z]^{-1} Z'X_sR^{[2]}.$$

But since the original design matrix was rotatable this implies

$$X_s' Z[Z'Z]^{-1} Z'X_s = R^{[2]} X'_s Z[Z'Z]^{-1} Z'X_sR^{[2]}.$$

To find the conditions this imposes on the block moment components, we will define the vector $\underline{t} = [1 \quad t_1 \quad t_2 \quad \ldots \quad t_k]$ and the generating function

$$Q = \underline{t}'^{[2]} P_s \underline{t}^{[2]}$$

where

$$P_s = X_s' Z[Z'Z]^{-1} Z'X_s.$$

Then if we define $\underline{u} = R\underline{t}$ and impose the requirement

$$Q = \underline{t}'^{[2]} P_s t^{[2]} = \underline{t}'^{[2]} R'P_s R\underline{t}^{[2]} = \underline{u}'^{[2]} P_s \underline{u}^{[2]}$$

this implies that Q must be a function of $\underline{u}'\underline{u} = \underline{t}'\underline{t} = \rho^2$ only, since Q is invariant in the k dimensional space of $t_1, t_2, \ldots, t_k$ under a general rotation to new axes $u_1, u_2, \ldots, u_k$. Hence, since Q is a polynomial of fourth degree in the t_i, it must be of the form

$$Q = a_o + a_2 \sum_i^k t_i^2 + a_4 (\sum_i^k t_i^2)^2 .$$

The conditions on the block moments can now be obtained by expanding the quadratic form $\underline{t}'^{[2]} P_s \underline{t}^{[2]}$ and equating the coefficients.

Inverting Z'Z (25) and performing the necessary algebra, we have

$$Z[Z'Z]^{-1}Z' = \left[\begin{array}{c|c|c|c} (\frac{1}{n_1} - \frac{1}{N})\underline{1}_{n_1}\underline{1}'_{n_1} & -\frac{1}{N}\underline{1}_{n_1}\underline{1}'_{n_2} & \cdots & -\frac{1}{N}\underline{1}_{n_1}\underline{1}'_{n_m} \\ \hline -\frac{1}{N}\underline{1}_{n_2}\underline{1}'_{n_1} & (\frac{1}{n_2} - \frac{1}{N})\underline{1}_{n_2}\underline{1}'_{n_2} & \cdots & -\frac{1}{N}\underline{1}_{n_2}\underline{1}'_{n_m} \\ \hline \cdots & \cdots & \cdots & \cdots \\ \hline -\frac{1}{N}\underline{1}_{n_m}\underline{1}'_{n_1} & -\frac{1}{N}\underline{1}_{n_m}\underline{1}'_{n_2} & & (\frac{1}{n_m} - \frac{1}{N})\underline{1}_{n_m}\underline{1}'_{n_m} \end{array}\right]_{N \text{ by } N}$$

and partitioning P_s into constant, quadratic, linear and interaction submatrices we have

$$P_s = N^2 \left[\begin{array}{c|c|c|c} 0 & \underline{0}'_k & \underline{0}'_k & \underline{0}'_{\binom{k}{2}} \\ \hline \underline{0}_k & P_{22} & \sqrt{2}\ P_{21} & \sqrt{2}\ P_{2(11)} \\ \hline \underline{0}_k & \sqrt{2}\ P'_{21} & 2\ P_{11} & 2\ P_{1(11)} \\ \hline \underline{0}_{\binom{k}{2}} & \sqrt{2}\ P'_{2(11)} & 2\ P'_{1(11)} & 2\ P_{(11)(11)} \end{array}\right]_{\binom{k+2}{2} \text{ by } \binom{k+2}{2}}$$

where the element in the i^{th} row and j^{th} column of the submatrix

$$P_{22} \text{ is } \sum_{w=1}^{m} \frac{[i^2]_{bw}\,[j^2]_{bw}}{n_w} - \frac{\lambda_2^2}{N}, \quad i, j = 1, 2, \ldots k$$

$$P_{21} \text{ is } \sum_{w=1}^{m} \frac{[i^2]_{bw}\,[j]_{bw}}{n_w}, \quad i, j = 1, 2, \ldots k$$

$$P_{2(11)} \text{ is } \sum_{w=1}^{m} \frac{[i^2]_{bw}\,[jj']_{bw}}{n_w}, \quad \begin{array}{l} i = 1, 2, \ldots k \\ jj' = 12, 13, \ldots (k-1)k \end{array}$$

$$P_{11} \text{ is } \sum_{w=1}^{m} \frac{[i]_{bw}\,[j]_{bw}}{n_w}, \quad i, j = 1, 2, \ldots k$$

$$P_{(11)(11)} \text{ is } \sum_{w=1}^{m} \frac{[ii']_{bw}\,[jj']_{bw}}{n_w}, \quad ii', jj' = 12, 13, \ldots (k-1)k.$$

The factors $\sqrt{2}$ and 2 arise in P_s since we will express the moment conditions in terms of the elements of P rather than of P_s.

After expanding Q and equating coefficients, we find that ten conditions must be satisfied if rotatable variance contours are to be retained after using non-orthogonal blocking with any rotatable design. In the following, all summations are over $w = 1, 2, \ldots m$.

1. $\sum \frac{[i^2]^2_{bw}}{n_w} = \text{constant}, \quad i = 1, 2 \ldots k$

2. $\sum \frac{[i^2]^2_{bw}}{n_w} = \sum \frac{[i^2]_{bw}\,[j^2]_{bw}}{n_w} + 2\sum \frac{[ij]^2_{bw}}{n_w}, \quad i \neq j$

3. $\sum \frac{[i]^2_{bw}}{n_w} = \text{constant}, \quad i = 1, 2 \ldots k$

4. $\sum \frac{[i]_{bw}\,[j]_{bw}}{n_w} = 0, \quad i \neq j$

5. $\sum \frac{[i^2]_{bw}\,[i]_{bw}}{n_w} = 0, \qquad i = 1, 2 \ldots k$

6. $\sum \frac{[i^2]_{bw}\,[j]_{bw}}{n_w} = -2\sum \frac{[i]_{bw}\,[ij]_{bw}}{n_w}, \qquad i \neq j$

7. $\sum \frac{[i]_{bw}\,[j\ell]_{bw}}{n_w} = 0, \qquad i \neq j \neq \ell$

8. $\sum \frac{[i^2]_{bw}\,[ij]_{bw}}{n_w} = 0, \qquad i \neq j$

9. $\sum \frac{[i^2]_{bw}\,[j\ell]_{bw}}{n_w} = -\sum \frac{[ij]_{bw}\,[i\ell]_{bw}}{n_w}, \qquad i \neq j \neq \ell$

10. $\sum \frac{[ij]_{bw}\,[\ell m]_{bw}}{n_w} = 0, \qquad i \neq j \neq \ell \neq m.$

It can be noted that no direct restrictions are placed on the individual moment components $[i]_{bw}$, $[i^2]_{bw}$ and $[ij]_{bw}$ by these ten conditions although they may be implied unless m is large. However, it is reasonable in many instances to use blocks which are first order rotatable, i.e., blocks for which

$$[i^2]_{bw} = \text{constant for } i = 1, 2, \ldots k$$
$$[i]_{bw} = 0$$
$$[ij]_{bw} = 0$$

Substituting these restrictions in the ten general conditions, we see that whenever blocks are first order rotatable the use of non-orthogonal blocking will not disturb the rotatability of an already rotatable design.

10.3.2 General Solution for Regression Coefficients and Their Variances - Blocks First Order Rotatable. From the preceding section we have the general form of the left hand side of the adjusted normal equations as $\overset{\circ}{X}'\overset{\circ}{X} = X'X - P$. The right hand side of the equation $\overset{\circ}{X}'\underline{y} = X'\underline{y} - Z[Z'Z]^{-1} Z'\underline{y}$ is easily found (utilizing the general form of $Z[Z'Z]^{-1} Z$ from 10.3.1) to be

$$\overset{\bullet}{X}'\underline{y} = \begin{bmatrix} \{oy\} \\ \hline \vdots \\ \{iiy\} - N\sum_{w=1}^{m} [i^2]_{bw}\, \bar{y}_w + \lambda_2 \{oy\} \\ \vdots \\ \hline \vdots \\ \{iy\} - N\sum_{w=1}^{m} [i]_{bw}\, \bar{y}_w \\ \vdots \\ \hline \vdots \\ \{ijy\} - N\sum_{w=1}^{m} [ij]_{bw}\, \bar{y}_w \\ \vdots \end{bmatrix}$$

where $\bar{y}_w$ is the mean of all observations in block w, and we use the notation

$$\{oy\} = \sum_{u=1}^{N} y_u, \quad \{iy\} = \sum_{u=1}^{N} x_{iu}y_u, \quad \{ijy\} = \sum_{u=1}^{N} x_{iu}x_{ju}y_u.$$

Since each submatrix of a simplex-sum design (D_s) is individually first order rotatable, we only require the general solution of these normal equations when $[i]_{bw} = [ij]_{bw} = 0$ and $[i^2]_{bw}$ is constant for all i, in order to provide solutions for any submatrix blocking scheme, $2 \leq m \leq k$. This greatly simplifies the solution since the elements of P_{22} all become $[\sum [i^2]_{bw}^2 / n_w - \lambda_2^2 / N]$ and the other elements of P vanish. Further, $\overset{\circ}{X}'\underline{y}$ differs from $X'\underline{y}$ only by the constant correction factor subtracted from the k elements in the quadratic portion i.e., $[N\sum [i^2]_{bw}\, \bar{y}_w - \lambda_2 \{ oy \}]$. Hence only the estimates of the quadratic

(b_{ii}) and correlated b_o coefficients will be affected by this particular kind of non-orthogonality. The estimates of the linear (b_i) and interaction (b_{ij}) coefficients are unaffected since they are in fact orthogonal to blocks, so that the general formulas given in (12) apply.

The general form of the information matrix when blocks are first order rotatable, in terms of unstandardized units, is given by

$$N[\dot{X}'\dot{X}]^{-1} = \left[\begin{array}{c|cccc|c|c} c_o & & c_1 \underline{1}'_k & & & 0 & 0 \\ \hline & c_{11} & c_{12} & \cdots & c_{12} & & \\ c_1 \underline{1}_k & c_{12} & c_{11} & \cdots & c_{12} & 0 & 0 \\ & \cdots & & \cdots & & & \\ & c_{12} & c_{12} & \cdots & c_{11} & & \\ \hline 0 & & 0 & & & \frac{1}{\lambda_2} I_k & 0 \\ \hline 0 & & 0 & & & & \frac{1}{\lambda_4} I_{\binom{n}{2}} \end{array}\right]$$

where

$$c_o = 2\lambda_4 A_\alpha [(k+2)\lambda_4 - k(N\sum \frac{[i^2]^2_{bw}}{n_w} - \lambda_2^2)] ,$$

$$c_1 = -2\lambda_4 \lambda_2 A_\alpha ,$$

$$c_{11} = A_\alpha [(k+1)\lambda_4 - (k-1) N \sum \frac{[i^2]^2_{bw}}{n_w}] ,$$

$$c_{12} = A_\alpha [N \sum \frac{[i^2]^2_{bw}}{n_w} - \lambda_4] ,$$

$$A_\alpha^{-1} = 2\lambda_4 [(k+2)\lambda_4 - k N \sum \frac{[i^2]^2_{bw}}{n_w}] ,$$

and 0 represents a null submatrix of suitable size.

Since under orthogonal blocking

$$[i^2]_{bw} = n_w \ \lambda_2/N$$

it is readily seen that in this case the information matrix collapses to the usual standard form (12) for a rotatable design.

The estimates of the regression coefficients may be written as

$$b_o = N^{-1} [\{oy\} - 2A_\alpha \lambda_4 \lambda_2 (\sum_i^k \{iiy\} - k \ N \sum_w^m [i^2]_{bw} \ \bar{\bar{y}}_w)]$$

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

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

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

Their variances and covariances are obtained easily from the information matrix. The variance of an estimated response may be written as

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

The variance function defined in (12) as $V(\rho) = (N/\sigma^2) \ V(\hat{y})$ for standardized variables, <u>i.e.,</u> $\sum_u x_{iu}^2 = N$, becomes

$$V(\rho) = A_\alpha \Big\{ 2(k+2)\lambda_4^2 - 2k \ \lambda_4 (N \sum \frac{[i^2]_{bw}^2}{n_w} - 1) + 2\lambda_4 [(k+2)\lambda_4$$
$$- (k \ N \sum \frac{[i^2]_{bw}^2}{n_w} + 2)] \ \rho^2 + [(k+1) \ \lambda_4 - (k-1) \ N \sum \frac{[i^2]_{bw}^2}{n_w}] \ \rho^4 \Big\}.$$

To gain an insight into the effect of departures from orthogonality on the variances of the estimates, we may define a "non-orthogonality parameter" (Δ_{iw}) as

$$\Delta_{iw} = \frac{[i^2]_{bw}}{\lambda_2} - \frac{n_w}{N} \qquad \begin{matrix} w = 1,\ 2\ \ldots\ m \\ i = 1,\ 2\ \ldots\ k \end{matrix}$$

For first order orthogonal blocking Δ_{iw} is constant for all i in a block and we may therefore dispense with the subscript i and use Δ_w as the block parameter.

Since

$$N \sum \frac{[i^2]_{bw}^2}{n_w} = \lambda_2^2\ [N \sum \frac{\Delta_w^2}{n_w} + 1]$$

we may write

$$V(b_{ii}) = \frac{(k+1)\ \lambda_4 - (k-1)\ \lambda_2^2\ (N \sum \frac{\Delta_w^2}{n_w} + 1)}{2\lambda_4 N[(k+2)\ \lambda_4 - k\ \lambda_2^2\ (N \sum \frac{\Delta_w^2}{n_w} + 1)]}$$

$$V(b_o) = \frac{(k+2)\ \lambda_4 - k\ \lambda_2^2\ N \sum \frac{\Delta_w^2}{n_w}}{N[(k+2)\ \lambda_4 - k\ \lambda_2^2\ (N \sum \frac{\Delta_w^2}{n_w} + 1)]}$$

If we let $\Theta = \sum \frac{\Delta_w^2}{n_w}$, $(0 \leq \Theta)$ and differentiate to find the rate of change of $V(b_{ii})$, for example, with respect to Θ we have

$$\frac{\partial V(b_{ii})}{\partial \Theta} = \frac{\lambda_2^2}{[(k+2)\ \lambda_4 - k\ \lambda_2^2\ (N\ \Theta + 1)]^2}\ .$$

Hence, since the slope is strictly positive we have that $V(b_{ii})$ is minimum at $\Theta = 0$ (i.e., when the blocking is orthogonal) and is monotonically increasing as Θ increases. Similarly

$$\frac{\partial V(b_o)}{\partial \Theta} = \frac{k^2\ \lambda_2^4}{[(k+2)\ \lambda_4 - k\ \lambda_2^2\ (N\ \Theta + 1)]^2}\ .$$

(The slopes must remain finite under our original assumption that the model is of full rank since the denominator is the same as that of the elements of the information matrix.)

The magnitudes of the Δ_w for the standard solution submatrix blocks are listed below when center points have been added to approach uniform variance. These values will serve to indicate the magnitude of the parameters since the specific solution Δ_w are of the same order.

Table 8. Non-orthogonality parameters for submatrix blocks

k	Δ_1	Δ_2	Δ_3	Δ_4	Δ_5	Δ_6	Δ_7	Δ_8
3	-.0071	.0142	-.0071					
4	.0012	-.0012	-.0012	.0012				
5	.0021	.0041	-.0124	.0041	.0021			
6	-.0012	-.0021	.0032	.0032	-.0021	-.0012		
7	.0012	.0003	-.0018	.0006	-.0018	.0003	.0012	
8	.0004	.0002	.0003	-.0009	-.0009	.0003	.0002	.0004

The tabled values also illustrate the properties of the Δ_w that are evident from the formulas, i.e.,

$$\sum_{w=1}^{m} \Delta_w = 0 ,$$

and for symmetric blocks,

$$\Delta_w = \Delta_{m-w} .$$

11.0 A CONVENIENT REDUCED DESIGN FOR k = 7

The design derived from the basis vector, γ_3 for the seven factor design in Section 8.2, 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 (12) requires 78 points (plus center points).

11.1 Construction

The vector of radius multipliers which defines this design is

$$\underline{a} = (0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0)'$$

and thus utilizes the points specified by the matrices D_2 and D_6 only.

In seven dimensions it is possible to find a matrix D_1, giving the coordinates of a regular simplex, which involves only the two levels -1 and +1, for each factor. Consequently D_2 and D_6 will only involve three factor levels. This design is therefore a desirable one from the standpoint of the experimenter who, as a result of physical or financial problems, is often forced to keep the number of different levels of each factor to a minimum. It will also be recalled that D_2 and D_6 form orthogonal blocks.

The 8 x 8 matrix $[\underline{1}\ D_1]$ 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 $\frac{1}{2} D_2$ and $\frac{1}{2} D_6$ are shown in Table 9. Since multiplication by a constant is permissible, we will define our derived design matrix D therefore as

$$D = \begin{bmatrix} \frac{1}{2} D_2 \\ \\ \frac{1}{2} D_6 \end{bmatrix} .$$

Table 9. Seven factor second order rotatable design in three levels

½ D_2							½ D_6						
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

Obtaining λ_4' either directly or, as shown below, via the general formulas, we have

$$[i^2j^2] = \lambda_4 = \sum a_s^4 \binom{n-4}{s-2} \frac{n^2}{N} = \frac{1}{7}$$

$$[i^2] \quad = \lambda_2 = \sum a_s^2 \binom{n-2}{s-1} \frac{n}{N} = \frac{3}{7}$$

$$\lambda_4' \quad = \frac{\lambda_4}{\lambda_2^2} = \frac{7}{9}$$

The singular value $\frac{k}{k+2}$ equals $\frac{7}{9}$ also and hence this design requires center points in order to make it possible to estimate all coefficients separately. The singularity is readily detectable also by noting that all design points lie on the hypershere of radius $\sqrt{3}$.

11.2 Projection Into Lesser Dimensionality

Orthogonal projections of this design into lesser dimensionality will also provide second order rotatable designs. Projections parallel to one or more design axes provide simple, easily obtained designs.

Taking as an example the projections of this type into three space we find that two distinct designs result. The first is typified by the projection on the axes of columns 1, 2 and 4 of D (parallel to axes 3, 5, 6, 7) and turns out to be precisely the design obtained in Section 9. In this design eight replicates of a_2D_2 were taken resulting in the cube with vertices at all permutations of $(\pm 1 \pm 1 \pm 1)$ and eight replicates on each of the faces at $(\pm 1\ 0\ 0)$, $(0 \pm 1\ 0)$ and $(0\ 0 \pm 1)$.

The second projection is typified by taking the coordinates of columns 1, 2 and 3 (projection parallel to axes 4, 5, 6, 7). Here we obtain from a_2D_2 the vertices of a cuboctahedron, i.e., the points at the midpoints of the edges of the cube obtained above. Inside this figure, with vertices at the midpoints of the faces of the cube, are two replicates of an octahedron, and, finally, four center points. These twenty-eight points from D_2 superimpose on those from D_6 and hence only one set is required. A three level second order rotatable design is thus obtained requiring twenty-eight points. The projection of the design inherits the same value of λ_4' but the moment matrix is no longer singular since k has changed.

$$\lambda_4' = \frac{7}{9} = .778$$

$$\frac{k}{k+2} = \frac{3}{5} = .600$$

11.3 Relation to 3^7 Design

It is interesting to note that this seven factor design matrix

$$D = \begin{bmatrix} \frac{1}{2} D_2 \\ \frac{1}{2} D_6 \end{bmatrix}$$

is a piece (or improper fractional replicate, since it is a $\frac{56}{3^7}$) of a 3^7 design which, after adding sufficient center points, gives estimates of all second order terms. Its projections into lesser dimensionality will yield 3^k designs ($k < 7$) with similar properties if orthogonal projections parallel to sets of design axes are used. The matrices D_3 and D_5 give pieces of a 4^7 design (each is a $\frac{56}{4^7}$ replicate) since the values 3, 1, -1, -3 are generated. In this case, however, we have shown that second order rotatability cannot be achieved without adding D_1 and D_7 to the matrix. D_3 and D_5 by themselves, however, have orthogonal columns and are, therefore, useful designs in their own right.

Future work may show this to be a fruitful way of obtaining useful pieces of factorial designs.

12.0 SUMMARY

It has been shown that second order rotatable designs in k factors can be generated by using the k + 1 rows of any minimum k factor first order rotatable design matrix as a generating set. The required first order design matrix is easily obtained by taking any matrix with k orthogonal columns and n = k + 1 rows, normalizing the length of the column vectors to $\sqrt{n}$, and removing the column means from the elements of each column. Calling this matrix D_1, the additional matrices $D_2, D_3, \ldots, D_s, \ldots, D_k$ can be generated where each D_s is an $\binom{n}{s}$ by k matrix whose row vectors consist of all possible sums of the rows of D_1 taken s at a time. Defining the N by k design matrix D, $(N = 2^n - 2)$ as

$$D = \begin{bmatrix} a_1 D_1 \\ \hline a_2 D_2 \\ \hline \vdots \\ \hline a_s D_s \\ \hline \vdots \\ \hline a_k D_k \end{bmatrix}$$

it was shown that by suitable choice of the radius multipliers $a_1, a_2, \ldots, a_k$, the matrix D could be made to satisfy the moment conditions for second order rotatability.

A solution for the radius multipliers, called the standard solution, was found which holds generally for all k and requires that

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

Designs obtained from the standard solution, however, all require $2^n - 2$ points plus any added center points and hence for most applications these designs become excessively large as k increases above five. Additional designs, called reduced designs, were then found and tabulated for $k = 5, 6, 7, 8$. These were more conservative in the number of points required since some of the radius multipliers were zero allowing the corresponding submatrices to be omitted from the design matrix. General expressions for the radius multipliers of reduced designs were not given, but a simple procedure was outlined which could be used if designs in higher dimensions were desired. A means of obtaining additional designs for $5 \leq k \leq 8$ was also provided.

It was found that designs generated by this method did not satisfy the moment conditions for third order rotatability for $k \leq 8$.

A means of replicating submatrices arbitrary numbers of times, without destroying rotatability, was given. This provides an alternate means of obtaining an estimate of experimental error in the event that center point replication is not desired.

Blocking procedures, both orthogonal and nearly orthogonal, were provided for these designs. In connection with the latter blocking schemes, a general theorem was proved showing the block-moment conditions necessary to retain second order rotatability when the regression coefficients are estimated by least squares taking into account the non-orthogonal block effects. It was shown that if blocks were formed such that each was itself a first order rotatable design, this would be sufficient to insure rotatability. This implied that any submatrix $a_s D_s$ of the simplex-sum designs could be used as a block. General formulas for the regression coefficients and their variances were found under general conditions of non-orthogonal first order rotatable blocking.

An extremely efficient second order rotatable simplex-sum design for seven factors was discussed as an illustration requiring only fifty-six points and three levels of each factor. It was shown that the projections of this design produced useful three level designs in lower dimensionality.

In order to obtain general expressions for the moments of simplex-sum designs, the moments of each submatrix were found as a function of the moments of D_1. Since the rows of D_1 can be regarded as the n vector elements of a finite k-variate population with orthogonal columns, it is readily seen that the expressions found are in essence sampling moments and as such may find wider application than considered here.

The voluminous algebra involved in deriving these moments was simplified considerably by using generalized bracket notation. In order to extend the use of this tool to multivariate populations it was demonstrated in Appendix A that the same rules used for taking averages or expectations in the univariate case apply for the multivariate generalizations.

Additional work is indicated in the direction of finding third order rotatable designs by methods similar to those described here. A study of the sixth order moments leads one to suspect that third order conditions can be met by introducing additional flexibility into the method by some means. The introduction of further submatrices by additional vector summing is a possible candidate.

In the interest of completeness, the derivation of the missing fifth and sixth order moments, which were not required here, would prove useful in sampling applications as well as in a further investigation of third order rotatability.

One other avenue of investigation suggested by this dissertation was the possibility of generating useful portions of factorial designs by simplex-sum or related procedures. As discussed in the final chapter, the fifty-six point design for seven factors can be considered as a piece of a 3^7 factorial. Although not the usual sort of fraction it is extremely efficient in estimating all second degree coefficients after adding center points to the basic design. Some additional investigations along these lines are discussed in (7).

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APPENDIX

APPENDIX A

MULTIVARIATE BRACKETS

Following Tukey's notation (26) let us define expressions called "brackets" as follows for the scalar (univariate) case:

$$\langle p \rangle = \frac{\sum_{i=1}^{s} x_i^p}{s}$$

$$\langle p_1 p_2 \rangle = \frac{\sum_{i,j}^{s\,\neq} x_i^{p_1} x_j^{p_2}}{s(s-1)}$$

$$\langle p_1 p_2 \cdots p_m \rangle = \frac{\sum_{i,j,\ldots,q}^{s\,\neq} x_i^{p_1} x_j^{p_2} \ldots x_q^{p_m}}{s(s-1)\ \ldots\ (s-m+1)}$$

where the summation takes place over unequal indices and the denominator consists of the total number of terms in the numerator. These expressions are "inherited on the average" which is to say that their average or expectation over all samples of size s is equal to the same function of the n population elements.

$$\text{Ave}\ [\ \langle p_1 p_2 \cdots p_m \rangle\ ] = \langle p_1 p_2 \cdots p_m \rangle' = \frac{\sum_{i,j\ldots q}^{n\,\neq} x_i^{p_1} x_j^{p_2} \ldots x_q^{p_m}}{n(n-1)\ \ldots\ (n-m+1)}$$

In extending this notation to a bivariate population [x y] the bracket $\langle 1\ 2 \rangle$ for example, can take on several meanings. We shall, therefore, change our notation slightly such that

$$\langle x, y^2 \rangle = \frac{\sum^{s \neq} x_i y_j^2}{s(s-1)}$$

$$\langle x, xy \rangle = \frac{\sum^{s \neq} x_i x_j y_j}{s(s-1)}$$

These brackets will be the bivariate equivalent of the univariate $\langle 1\ 2 \rangle$ bracket. An obvious extension of this principle yields multivariate brackets of any desired order.

To demonstrate that these brackets are also inherited on the average we will first consider the bivariate case. Let $z_i = x_i + y_i$, then

$$\left[\frac{\sum_{i=1}^{s} z_i}{s}\right]^2 = \frac{\sum_i^s z_i^2}{s^2} + \frac{\sum_{i,j}^{s \neq} z_i z_j}{s^2} \quad \text{or} \quad \langle z \rangle^2 = \frac{1}{s}\langle z^2 \rangle + \frac{(s-1)}{s}\langle z, z \rangle$$

and Ave $[\langle z \rangle^2] = \frac{1}{s}$ Ave $\langle z^2 \rangle + \frac{s-1}{s}$ Ave $\langle z, z \rangle = \frac{1}{s}\langle z^2 \rangle' + \frac{s-1}{s}\langle z, z \rangle'$.

But

$$\langle z^2 \rangle' = \frac{\sum (x_i + y_i)^2}{n} = \frac{\sum x_i^2 + \sum y_i^2 + 2\sum x_i y_i}{n}$$

$$= \langle x^2 \rangle' + \langle y^2 \rangle' + 2\langle xy \rangle',$$

and

$$\langle z, z \rangle' = \frac{\sum^{\neq}(x_i+y_i)(x_j+y_j)}{n(n-1)} = \frac{\sum^{\neq} x_i x_j + \sum^{\neq} y_i y_j + 2\sum^{\neq} x_i y_j}{n(n-1)}$$

$$= \langle x,x \rangle' + \langle y,y \rangle' + 2\langle x,y \rangle'.$$

Therefore

$$\text{Ave } [\langle z \rangle^2] = \frac{1}{s}(\langle x^2 \rangle' + \langle y^2 \rangle' + 2\langle xy \rangle') + \frac{(s-1)}{s}(\langle x,x \rangle'$$

$$+ \langle y,y \rangle' + 2\langle x,y \rangle').$$

Alternatively we may expand $\langle z \rangle^2$ before taking the average over all samples

$$\langle z \rangle^2 = \frac{1}{s}(\langle x^2 \rangle + \langle y^2 \rangle + 2\langle xy \rangle) + \frac{(s-1)}{s}(\langle x,x \rangle + \langle y,y \rangle + 2\langle x,y \rangle)$$

$$\text{Ave}\,[\langle z \rangle^2] = \frac{1}{s}(\text{Ave}\,[\langle x^2 \rangle] + \text{Ave}\,[\langle y^2 \rangle] + 2\,\text{Ave}\,[\langle x\,y \rangle] + \frac{(s-1)}{s}(\text{Ave}\,[\langle x,x \rangle] + \text{Ave}\,[\langle y,y \rangle] + 2\,\text{Ave}\,[\langle x,y \rangle]).$$

Recognizing $\text{Ave}\,[\langle xy \rangle] = \langle xy \rangle'$ since we can redefine $x_i y_i$ as a new population whose elements are $u_i = x_i y_i$ and use the univariate property of the brackets, we can write

$$\text{Ave}\,[\langle z \rangle^2] = \frac{1}{s}(\langle x^2 \rangle' + \langle y^2 \rangle' + 2\langle xy \rangle') + \frac{s-1}{s}(\langle x,x \rangle' + \langle y,y \rangle' + 2\,\text{Ave}\,[\langle x,y \rangle]).$$

Equating terms with the previously derived expression for $\text{Ave}\,[\langle z^2 \rangle]$ we see that

$$\text{Ave}\,[\langle x,y \rangle] = \langle x,y \rangle'.$$

By a similar series of operations we can begin with $\langle z \rangle^3$ and take the average before and after expanding in terms of x and y. We will then have upon equating terms

$$\text{Ave}\,[\langle x,x,y \rangle] + \text{Ave}\,[\langle x,y,y \rangle] = \langle x,x,y \rangle' + \langle x,y,y \rangle'$$

or

$$\text{Ave}\,[\langle x,x,y \rangle] - \langle x,x,y \rangle' + \text{Ave}\,[\langle x,y,y \rangle] - \langle x,y,y \rangle' = 0.$$

Since this equation holds for all values of x and y consider the two populations of n values

$$(\underline{x}\ \underline{y}) = (\underline{x}_1\ \underline{y}_1)$$

$$(\underline{x}\ \underline{y}) = (2\underline{x}_1\ \underline{y}_1).$$

Substituting in the above for each

$$\text{Ave}\ [\langle x_1,x_1,y_1\rangle] - \langle x_1,x_1,y_1\rangle' + \text{Ave}\ [\langle x_1,y_1,y_1\rangle]$$

$$- \langle x_1,y_1,y_1\rangle' = 0$$

and

$$4\ \text{Ave}\ [\langle x_1,x_1,y_1\rangle] - 4\langle x_1,x_1,y_1\rangle' + 2\ \text{Ave}\ [\langle x_1,y_1,y_1\rangle]$$

$$- 2\langle x_1,y_1,y_1\rangle' = 0.$$

If we define the vector $\underline{u} = [u_1\ u_2]'$ where

$$u_1 = \text{Ave}\ [\langle x_1,x_1,y_1\rangle] - \langle x_1,x_1,y_1\rangle'$$

$$u_2 = \text{Ave}\ [\langle x_1,y_1,y_1\rangle] - \langle x_1,y_1,y_1\rangle'$$

we can then consider these equations as two homogeneous equations in two unknowns

$$\begin{bmatrix} 1 & 1 \\ 4 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = 0 \quad .$$

Clearly, only the trivial solution, $\underline{u} = \underline{0}$, is possible since the coefficient matrix is non-singular. Therefore we can write

$$\text{Ave}\ [\langle x_1,x_1,y_1\rangle] = \langle x_1,x_1,y_1\rangle'$$

$$\text{Ave}\ [\ x_1,y_1,y_1\ ] = \langle x_1,y_1,y_1\rangle'.$$

This procedure can be extended step by step indefinitely for $\langle z \rangle^{\alpha}$ since the same function of the z_i's is obtained whether the average is taken before or after expanding in terms of x and y. As a consequence, upon equating terms all will cancel except those (α-1) terms of order α which equate in total and must then be proven equal term by term. A procedure corresponding to that just discussed for the case $\alpha = 2$ will lead to a set of homogeneous equations $A\underline{u} = \underline{0}$ with a non-singular coefficient matrix. We can therefore say in general that the bivariate brackets are inherited on the average.

To extend to trivariate brackets we let $z_i = w_i + x_i + y_i$ and proceed again in stepwise fashion beginning with $\langle z \rangle^3$ and proving Ave $[\langle w,x,y \rangle] = \langle w,y,z \rangle'$. It is evident therefore that multivariate brackets in general are inherited on the average since we can proceed in this manner to any order and any number of variables.

APPENDIX B

DERIVATION OF GENERAL MOMENT FORMULAS

B.1 Introduction

Using this convenient property of the bracket expressions it is possible to derive the general moment formulas for D_s. In finding the sampling moments of means of samples of s drawn from a univariate population of n we seek

$$\text{Ave}\ [(\frac{x_1 + x_2 + \ldots + x_s}{s})^{\alpha}] = \text{Ave}\ [\langle x \rangle^{\alpha}].$$

If we consider the n elements in the i-th column of D_1 as the population then the same column in D_s contains all possible sums of s from this population. Therefore

$$[i^{\alpha}]_s = \frac{1}{N} \sum_{1 \le u_1} \sum_{< u_2} \cdots \sum_{< u_k \le n} (x_{iu_1} + x_{iu_2} + \ldots + x_{iu_s})^{\alpha}$$

$$= N^{-1} s^{\alpha} \binom{n}{s}\ \text{Ave}\ [\langle x \rangle^{\alpha}]$$

where Ave $[\langle x \rangle^{\alpha}]$ must be multiplied by s^{α} because $[i^{\alpha}]_s$ involves sums, not means, and by $\binom{n}{s}$ to bring the average value up to the total moment of all $\binom{n}{s}$ terms. We may write in general then

$$[1^{\alpha_1}\ 2^{\alpha_2} \ldots k^{\alpha_k}]_s = N^{-1} s^{\alpha} \binom{n}{s}\ \text{Ave}\ [\langle x_1 \rangle^{\alpha_1} \langle x_2 \rangle^{\alpha_2} \ldots \langle x_k \rangle^{\alpha_k}]$$

where the general row vector of D_1 is considered as the k-variate vector $(x_{1u}\ x_{2u} \ldots x_{ku})$ and Ave $[\langle x_1 \rangle^{\alpha_1} \langle x_2 \rangle^{\alpha_2} \ldots \langle x_k \rangle^{\alpha_k}]$ represents its sampling moments. We denote the order of the moment by $\alpha = \sum \alpha_i$.

The bracket notation previously adopted therefore is conveniently usable in the same context, where $\langle x_i \rangle$ denotes summation over an arbitrary sample of s rows and $\langle x_i \rangle'$ sums over the entire column of n rows.

To find $[i]_s$ we proceed as follows:

$$[i]_s = N^{-1}s\binom{n}{s} \text{ Ave } [\langle x_i \rangle],$$

$$\text{Ave } [\langle x_i \rangle] = \langle x_i \rangle' = \frac{\sum x_{iu}}{n} = 0,$$

$$[i]_s = 0.$$

B.2 Second Order Moments

Similarly,

$$[ij]_s = N^{-1}s^2\binom{n}{s} \text{ Ave } [\langle x_i \rangle \langle x_j \rangle],$$

$$\text{Ave } [\langle x_i \rangle \langle x_j \rangle] = \text{Ave } [\frac{(x_{i1} + x_{i2} + \dots x_{is})}{s} \frac{(x_{j1} + x_{j2} + \dots + x_{js})}{s}]$$

$$= \frac{1}{s} \text{ Ave } [\frac{\sum_{u}^{s} x_{iu}x_{ju}}{s} + (s-1) \frac{\sum_{u,v}^{s\,\neq} x_{iu}x_{jv}}{s(s-1)}]$$

$$= \frac{1}{s} \text{ Ave } [\langle x_i x_j \rangle + (s-1)\langle x_i, x_j \rangle]$$

$$= \frac{1}{s} (\langle x_i x_j \rangle' + (s-1)\langle x_i, x_j \rangle').$$

In all summations that follow we shall sum from 1 to n over each of the second subscripts, (u, v, t, etc.) unless otherwise indicated.

$$\langle x_i x_j \rangle' = \frac{\sum x_{iu} x_{ju}}{n} = 0,$$

$$\langle x_i , x_j \rangle' = \frac{\sum^{\neq} x_{iu} x_{jv}}{n(n-1)} = \frac{\sum x_{iu} \sum x_{ju} - \sum x_{iu} x_{ju}}{n(n-1)} = 0,$$

$$[ij]_s = 0.$$

The final step of expanding the brackets into single index summations, i.e., in terms of the moments of D_1, can be accomplished most easily for the more complex summations which occur in the higher moments by using tables of symmetric functions (16). These tables provide formulas for the univariate summations only but are extremely helpful for writing out their multivariate generalizations. Illustrations of this will appear in the derivations which follow.

$$[i^2]_s = N^{-1} s^2 \binom{n}{s} \text{ Ave } [\langle x_i \rangle^2],$$

$$\text{Ave } [\langle x_i \rangle^2] = \text{Ave } [(\frac{x_{i1} + x_{i2} + \dots + x_{is}}{s})^2]$$

$$= \text{Ave } [\frac{1}{s} \langle x_i^2 \rangle + \frac{(s-1)}{s} \langle x_i , x_i \rangle]$$

$$= \frac{1}{s} \langle x_i^2 \rangle' + \frac{s-1}{s} \langle x_i , x_i \rangle'.$$

$$\langle x_i^2 \rangle' = \frac{\sum x_{iu}^2}{n} = \frac{n}{n} = 1,$$

$$\langle x_i, x_i \rangle' = \frac{\sum^{\neq} x_{iu}x_{iv}}{n(n-1)} = \frac{\sum x_{iu} \sum x_{iv} - \sum x_{iu}^2}{n(n-1)} = \frac{-n}{n(n-1)} = -\frac{1}{n-1},$$

$$\text{Ave } [\langle x_i \rangle^2] = \frac{1}{s} - \frac{s-1}{s(n-1} = \frac{n-s}{s(n-1)},$$

$$[i^2]_s = N^{-1}s^2 \frac{n!}{s!(n-s)!} \frac{n-s}{s(n-1)} = N^{-1}\binom{n-2}{s-2}n.$$

Or, in the more general case where $\sum x_{iu}^2$ has not been standardized to equal n,

$$[i^2]_s = N^{-1}\binom{n-2}{s-1} N[i^2]_1 = \binom{n-2}{s-1}[i^2]_1.$$

B.3 Third Order Moments

The general third order moment $[ijk]_s$ can be derived in the following manner

$$[ijk]_s = N^{-1}s^3\binom{n}{s} \text{ Ave } [\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle]$$

$$\text{Ave } [\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle] = \frac{1}{s^2} (\text{Ave } [\langle x_i x_j x_k \rangle + (s-1)(\langle x_i, x_j x_k \rangle$$

$$+ \langle x_j, x_i x_k \rangle + \langle x_k, x_i x_j \rangle) + (s-1)(s-2) \langle x_i, x_j, x_k \rangle])$$

$$= \frac{1}{s^2} [\langle x_i x_j x_k \rangle' + (s-1)(\langle x_i, x_j x_k \rangle'$$

$$+ \langle x_j, x_i x_k \rangle' + \langle x_k, x_i x_j \rangle') + (s-1)(s-2) \langle x_i, x_j, x_k \rangle'].$$

Utilizing tables of symmetric functions (16) to expand the brackets

$$\langle x_i x_j x_k \rangle' = \frac{\sum x_{iu} x_{ju} x_{ku}}{n} = \frac{N}{n}[ijk]_1,$$

$$\langle x_i, x_j x_k \rangle' = \frac{\sum^{\neq} x_{iu} x_{jv} x_{kv}}{n(n-1)} = \frac{\sum x_{iu} \sum x_{iu} x_{ku} - \sum x_{iu} x_{ju} x_{ku}}{n(n-1)}$$

$$= -\frac{N}{n(n-1)}[ijk]_1,$$

$$\langle x_j, x_i x_k \rangle' = -\frac{N}{n(n-1)}[ijk]_1,$$

$$\langle x_k, x_i x_j \rangle' = -\frac{N}{n(n-1)}[ijk]_1,$$

$$\langle x_i, x_j, x_k \rangle' = \frac{\sum^{\neq} x_{iu} x_{jv} x_{kt}}{n(n-1)(n-2)}$$

$$= \frac{1}{n(n-1)(n-2)} [\sum x_{iu} \sum x_{ju} \sum x_{ku} - (\sum x_{iu} x_{ju} \sum x_{ku}$$

$$+ \sum x_{iu} x_{ku} \sum x_{ju} + \sum x_{ju} x_{ku} \sum x_{iu}) + 2 \sum x_{iu} x_{ju} x_{ku}]$$

$$= \frac{2N}{n(n-1)(n-2)} [ijk]_1,$$

$$\text{Ave } [\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle] = \frac{N}{s^2}\left(\frac{1}{n} - \frac{3(s-1)}{n(n-1)} + \frac{2(s-1)(s-2)}{n(n-1)(n-2)}\right)[ijk]_1$$

$$= \frac{N(n-s)(n-2s)}{s^2 n(n-1)(n-2)}[ijk]_1.$$

Substituting this result in the equation for $[ijk]_s$

$$[ijk]_s = N^{-1}s^3\binom{n}{s}\frac{N}{s^2}\frac{(n-s)(n-2s)}{n(n-1)(n-2)}[ijk]_1 = \frac{(n-2s)}{(n-2)}\binom{n-2}{s-1}[ijk]_1.$$

In the preceding derivation we have implicitly assumed that s (and hence n) is strictly greater than 2 since $\langle x_i, x_j, x_k \rangle$ does not exist for s = 2. However it can be seen that after taking averages the unwanted term involving $\langle x_i, x_j, x_k \rangle'$ will vanish if we let s = 2 (or s = 1) since its coefficient (s-1)(s-2) vanishes provided $s < n$ and $n > 2$. In general we will follow this procedure where the expansion in terms of brackets will assume $s \geq \alpha$ (implying $n \geq \alpha$) in order to obtain the most general expression for the moment. The same argument holds however, _mutatis mutandis_, so that the formulas are valid for s = 1, 2, ..., n - 1 and $n \geq \alpha$. When s = n it is obvious that all moments vanish by the assumption of zero means. The only moments required here for $n < \alpha$ are the fourth order moments when n = 3 and these are treated separately.

To find $[ij^2]_s$ we follow the preceding derivation but let k = j.

$$[ij^2]_s = N^{-1}s^3\binom{n}{s} \text{ Ave } [\langle x_i \rangle \langle x_j \rangle^2],$$

$$\text{Ave } [\langle x_i \rangle \langle x_j \rangle^2] = \frac{1}{s^2}[\langle x_i x_j^2 \rangle' + (s-1)(\langle x_i, x_j^2 \rangle + 2\langle x_j, x_i x_j \rangle')$$

$$+ (s-1)(s-2)\langle x_i, x_j, x_j \rangle']$$

$$= \frac{N}{s^2}\left(\frac{1}{n} - \frac{3(s-1)}{n(n-1)} + \frac{2(s-1)(s-2)}{n(n-1)(n-2)}\right)[ij^2]_1.$$

Simplifying and substituting in the equation for $[ij^2]_s$

$$[ij^2]_s = \frac{(n-2s)}{(n-2)}\binom{n-2}{s-1}[ij^2]_1.$$

Similarly for $[i^3]_s$ let $k = j = i$.

$$[i^3]_s = N^{-1}s^3\binom{n}{s} \text{ Ave } [\langle x_i \rangle^3],$$

$$\text{Ave } [\langle x_i \rangle^3] = \frac{1}{s^2} [\langle x_i^3 \rangle' + 3(s-1) \langle x_i, x_i^2 \rangle' + (s-1)(s-2) \langle x_i, x_i, x_i \rangle'],$$

$$= \frac{N}{s^2} [\frac{1}{n} - \frac{3(s-1)}{n(n-1)} + \frac{2(s-1)(s-2)}{n(n-1)(n-2)}] [i^3]_1.$$

Substituting this result we then have

$$[i^3]_s = \frac{n-2s}{n-2} \binom{n-2}{s-1} [i^3]_1.$$

B.4 Fourth Order Moments

The fourth order moments may be derived in a similar fashion by first obtaining the general result $[ijkl]_s$.

$$[ijkl]_s = N^{-1}s^4\binom{n}{s} \text{ Ave } [\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle \langle x_l \rangle],$$

$$\text{Ave } [\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle \langle x_l \rangle] = \frac{1}{s^3}[\langle x_i x_j x_k x_l \rangle' + (s-1)(\langle x_i, x_j x_k x_l \rangle'$$

$$+ \langle x_j, x_i x_k x_l \rangle' + \langle x_k, x_i x_j x_l \rangle' + \langle x_l, x_i x_j x_k \rangle' + \langle x_i x_j, x_k x_l \rangle'$$

$$+ \langle x_i x_k, x_j x_l \rangle' + \langle x_i x_l, x_j x_k \rangle') + (s-1)(s-2)(\langle x_i, x_j, x_k x_l \rangle'$$

$$+ \langle x_i, x_k, x_j x_l \rangle' + \langle x_i, x_l, x_j x_k \rangle' + \langle x_j, x_k, x_i x_l \rangle'$$

$$+ \langle x_j, x_l, x_i x_k \rangle' + \langle x_k, x_l, x_i x_j \rangle')$$

$$+ (s-1)(s-2)(s-3) \langle x_i, x_j, x_k, x_l \rangle'].$$

Using tables of symmetric functions to expand these brackets and omitting terms containing zero elements of the type $\sum x_{iu}$

$$\langle x_i x_j x_k x_l \rangle' = \frac{\sum x_{iu} x_{ju} x_{ku} x_{lu}}{n} = \frac{N}{n}[ijkl]_1,$$

$$\langle x_i, x_j x_k x_l \rangle' = \frac{-\sum x_{iu} x_{ju} x_{ku} x_{lu}}{n(n-1)} = \frac{-N}{n(n-1)}[ijkl]_1$$

(all permutations of i, j, k, l yield an identical result),

$$\langle x_i x_j, x_k x_l \rangle' = \frac{\sum x_{iu} x_{ju} \sum x_{ku} x_{lu} - \sum x_{iu} x_{ju} x_{ku} x_{lu}}{n(n-1)} = \frac{-N}{n(n-1)}[ijkl]_1$$

(for all permutations of subscripts),

$$\langle x_i, x_j, x_k x_l \rangle' = \frac{-\sum x_{iu} x_{ju} \sum x_{ku} x_{lu} + 2 \sum x_{iu} x_{ju} x_{ku} x_{lu}}{n(n-1)(n-2)}$$

$$= \frac{2N}{n(n-1)(n-2)}[ijkl]_1$$

(for all permutations of subscripts),

$$\langle x_i, x_j, x_k, x_l \rangle' = \frac{1}{n(n-1)(n-2)(n-3)} \left(\sum x_{iu} x_{ju} \sum x_{ku} x_{lu} + \sum x_{iu} x_{ku} \sum x_{ju} x_{lu} \right.$$

$$\left. + \sum x_{iu} x_{lu} \sum x_{ju} x_{ku} - 6 \sum x_{iu} x_{ju} x_{ku} x_{lu} \right)$$

$$= \frac{-6N}{n(n-1)(n-2)(n-3)}[ijkl]_1.$$

Sums of the type $\sum x_{iu} x_{ju} \sum x_{ku} x_{lu}$ were written down, even though equal to zero in this case, because for some other fourth order moments they will be non-zero.

$$\text{Ave } [\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle \langle x_l \rangle] = \frac{N}{s^3}\Big[\frac{1}{n} - \frac{7(s-1)}{n(n-1)} + \frac{12(s-1)(s-2)}{n(n-1)(n-2)}$$

$$- \frac{6(s-1)(s-2)(s-3)}{n(n-1)(n-2)(n-3)}\Big] [ijkl]_1$$

$$= \frac{N}{s^3}\Big[\frac{(n-s)(n^2 + n - 6sn + 6s^2)}{n(n-1)(n-2)(n-3)}\Big][ijkl]_1$$

$$= \frac{N(n-s)[(n-2s)(n-3s) - n(s-1)]}{s^3 n(n-1)(n-2)(n-3)}[ijkl]_1 .$$

Upon substitution in the equation for $[ijkl]_s$ we have

$$[ijkl]_s = \Big[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\Big] \binom{n-2}{s-1}[ijkl]_1 .$$

In order to obtain $[ijk^2]_s$ let $l = k$ in the foregoing derivation.

$$[ijk^2]_s = N^{-1}s^4\binom{n}{s} \text{ Ave } [\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle^2].$$

Upon substituting for the brackets in Ave $[\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle^2]$ it is clear that the same coefficients will be obtained as in Ave $[\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle \langle x_l \rangle]$. No other term will be introduced since the expressions $\sum x_{iu}x_{ju} \sum x_{ku}^2 = \sum x_{iu}x_{ku} \sum x_{ju}x_{ku} = 0$ as before.

Therefore referring to the expression for $[ijkl]_s$ we can write

$$[ijk^2]_s = \Big[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\Big] \binom{n-2}{s-1}[ijk^2]_1 .$$

To obtain $[ij^3]_s$ we let $k = l = j$ in the first derivation. Then

$$[ij^3]_s = N^{-1}s^4\binom{n}{s} \text{ Ave } [\langle x_i \rangle \langle x_j \rangle^3].$$

Inspection of the expanded brackets listed for the $[ijkl]_s$ moment, keeping in mind the revised subscripts, again shows that the coefficients will be unchanged. The expression $\sum x_{iu}x_{ju}\sum x_{ju}^2 = 0$, hence no additional term appears. Utilizing the previous algebra we can write

$$[ij^3]_s = \left[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\right] \binom{n-2}{s-1} [ij^3]_1.$$

Another fourth-order moment is $[i^2j^2]_s$ which can be obtained by letting $k = i$ and $l = j$ in the derivation of $[ijkl]_s$.

$$[i^2j^2]_s = N^{-1}s^4\binom{n}{s} \text{ Ave } [\langle x_i \rangle^2 \langle x_j \rangle^2].$$

Again the same coefficient will be obtained for the $[i^2j^2]_1$ term in Ave $[\langle x_i^2 \rangle \langle x_j^2 \rangle]$ as was obtained in the three previous derivations for the corresponding terms. However a new term will be added to the moment due to the failure of the following terms to go to zero in the expansion of the brackets.

Expression	Added Term
$\langle x_i^2, x_j^2 \rangle'$	$\dfrac{\sum x_{iu}^2 \sum x_{ju}^2}{n(n-1)} = \dfrac{n}{n-1}$
$\langle x_i, x_i, x_j^2 \rangle'$	$\dfrac{-\sum x_{iu}^2 \sum x_{ju}^2}{n(n-1)(n-2)} = \dfrac{-n}{(n-1)(n-2)}$
$\langle x_j, x_j, x_i^2 \rangle'$	$\dfrac{-\sum x_{iu}^2 \sum x_{ju}^2}{n(n-1)(n-2)} = \dfrac{-n}{(n-1)(n-2)}$
$\langle x_i, x_i, x_j, x_j \rangle'$	$\dfrac{\sum x_{iu}^2 \sum x_{ju}^2}{n(n-1)(n-2)(n-3)} = \dfrac{n}{(n-1)(n-2)(n-3)}$

The additional term to be added to Ave $[\langle x_i \rangle^2 \langle x_j \rangle^2]$ therefore follows as

$$\frac{1}{s^3}\left[\frac{n(s-1)}{n-1} - \frac{2n(s-1)(s-2)}{(n-1)(n-2)} + \frac{n(s-1)(s-2)(s-3)}{(n-1)(n-2)(n-3)}\right] = \frac{1}{s^3}\left[\frac{(n-s)(s-1)(n-s-1)}{n(n-1)(n-2)(n-3)}\right] n^2.$$

Therefore

$$\text{Ave } [\langle x_i \rangle^2 \langle x_j \rangle^2] = \frac{N}{s^3}\Big[\frac{(n-2s)(n-3s) - n(s-1)}{n(n-1)(n-2)(n-3)}[i^2 j^2]_1$$

$$+ \frac{(n-s)(s-1)(n-s-1)}{n(n-1)(n-2)(n-3)} \; \frac{n^2}{N}\Big].$$

The last n^2 in the above expression can be replaced by $N^2[i^2]_1[j^2]_1$ for the more general case where the column vectors have not been standardized.

Substituting Ave $[\langle x_i \rangle^2 \langle x_j \rangle^2]$ in the expression for $[i^2 j^2]_s$ and simplifying we have

$$[i^2 j^2]_s = \Big[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\Big]\binom{n-2}{s-1}[i^2 j^2]_1 + \binom{n-4}{s-2}\frac{n^2}{N}$$

The final fourth order moment, $[i^4]_s$ is obtained easily from the result for $[i^2 j^2]_s$. The added terms in this case become

Expression	Added Term
$\langle x_i^2, x_i^2 \rangle'$	$\dfrac{\sum x_{iu}^2 \sum x_{iu}^2}{n(n-1)} = \dfrac{n}{n-1}$
$\langle x_i, x_i, x_i^2 \rangle'$	$\dfrac{-\sum x_{iu}^2 \sum x_{iu}^2}{n(n-1)(n-2)} = \dfrac{-n}{(n-1)(n-2)}$
$\langle x_i, x_i, x_i, x_i \rangle'$	$\dfrac{3\sum x_{iu}^2 \sum x_{iu}^2}{n(n-1)(n-2)(n-3)} = \dfrac{3n}{n(n-1)(n-2)(n-3)}$

The term $\langle x_i^2, x_i^2 \rangle'$ appears three times in the expansion of Ave $[\langle x_i \rangle^4]$. This can be readily seen by letting all subscripts equal i in the expansion of Ave $[\langle x_i \rangle \langle x_j \rangle \langle x_k \rangle \langle x_l \rangle]$. In the same way we see that

$\langle x_i, x_i, x_i^2 \rangle'$ appears six times and $\langle x_i, x_i, x_i, x_i \rangle'$ once. The coefficient of the additional term is therefore exactly three times that obtained for the previous case and

$$\text{Ave } [\langle x_i \rangle^4] = \frac{N}{s^3}\left[\frac{(n-2s)(n-3s) - n(s-1)}{n(n-1)(n-2)(n-3)}[i^4]_1 + 3\,\frac{(n-s)(s-1)(n-s-1)\;n^2}{n(n-1)(n-2)(n-3)}\right.$$

Therefore

$$[i^4]_s = \left[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\right]\binom{n-2}{s-1}[i^2j^2]_1 + 3\binom{n-4}{s-2}n^2$$

As in the preceding moment, the more general expression would be obtained by replacing the last n^2 by $N^2[i^2]_1^2$ for the case where $\sum x_{iu}^2 \neq n$.

B.5 Higher Order Moments

In order to determine whether a derived design is third order rotatable it is necessary to have its moments through the sixth order. However, due to the property demonstrated above, it is not necessary to obtain all the moments of any order to determine at least some multiple of the coefficients that are involved. For the purposes of this paper, then, it was unnecessary to derive all fifth and sixth order moments; in fact only three of the fifth order and two of the sixth order moments were obtained. The derivation of these moments will not be given as the procedure has already been outlined and the magnitude of the algebra makes it impractical to do so. Sixty-six different multivariate brackets are required to expand Ave $[\langle x_i \rangle^2 \langle x_j \rangle^2 \langle x_k \rangle^2]$ for example.

These results and those derived above are summarized in the following table.

Table 1. Moment components of totals of samples of s from zero mean finite orthogonal populations of n, $(n \geq \alpha)$

$$[i]_s = 0$$

$$[ij]_s = 0$$

$$[i^2]_s = \binom{n-2}{s-1}[i^2]_1$$

$$[ijk]_s = \frac{(n-2s)}{(n-2)}\binom{n-2}{s-1}[ijk]_1$$

$$[ij^2]_s = \frac{(n-2s)}{(n-2)}\binom{n-2}{s-1}[ij^2]_1$$

$$[i^3]_s = \frac{(n-2s)}{(n-2)}\binom{n-2}{s-1}[i^3]_1$$

$$[ijkl]_s = \left[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\right]\binom{n-2}{s-1}[ijkl]_1$$

$$[ijk^2]_s = \left[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\right]\binom{n-2}{s-1}[ijk^2]_1$$

$$[ij^3]_s = \left[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\right]\binom{n-2}{s-1}[ij^3]_1$$

$$[i^2j^2]_s = \left[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\right]\binom{n-2}{s-1}[i^2j^2]_1 + \binom{n-4}{s-2}[i^2]_1[j^2]_1\, N$$

$$[i^4]_s = \left[\frac{(n-2s)(n-3s) - n(s-1)}{(n-2)(n-3)}\right]\binom{n-2}{s-1}[i^4]_1 + 3\binom{n-4}{s-2}[i^2]_1^2\, N$$

$$[ijklm]_s = (n-2s)\left[\frac{(n-3s)(n-4s) - 5n(s-1)}{(n-2)(n-3)(n-4)}\right]\binom{n-2}{s-1}[ijklm]_1$$

$$[ijkl^2]_s = (n-2s)\left[\frac{(n-3s)(n-4s) - 5n(s-1)}{(n-2)(n-3)(n-4)}\right]\binom{n-2}{s-1}[ijkl^2]_1 + \frac{(n-2s)}{(n-4)}\binom{n-4}{s-2}[ijk]_1[l^2]_1\, N$$

$$[i^5]_s = (n-2s)\left[\frac{(n-3s)(n-4s) - 5n(s-1)}{(n-2)(n-3)(n-4)}\right]\binom{n-2}{s-1}[i^5]_1 + 10\frac{(n-2s)}{(n-4)}\binom{n-4}{s-2}[i^3]_1[i^2]_1\, N$$

$$[i^2j^2k^2]_s = \left[\frac{(n-2s)(n-3s)(n-4s)(n-5s) - n(s-1)(16n^2-79sn+11n+86s^2-4s-4)}{(n-2)(n-3)(n-4)(n-5)}\right]\binom{n-2}{s-1}[i^2j^2k^2]_1 + \left[\frac{n^2+3n-6ns+6s^2-4}{(n-4)(n-5)}\right]\binom{n-4}{s-2}\left([i^2j^2]_1[k^2]_1 + [i^2k^2]_1[j^2]_1 + [j^2k^2]_1[i^2]_1\right)N$$

$$+ 2\left[\frac{n^2-n-4sn+4s^2+4}{(n-4)(n-5)}\right]\binom{n-4}{s-2}\left([ij^2]_1[ik^2]_1 + [i^2j]_1[jk^2]_1 + [i^2k]_1[j^2k]_1 + 2[ijk]_1^2\right)N + \binom{n-6}{s-3}[i^2]_1[j^2]_1[k^2]_1\, N^2$$

$$[i^6]_s = \left[\frac{(n-2s)(n-3s)(n-4s)(n-5s) - n(s-1)(16n^2-79sn+11n+86s^2-4s-4)}{(n-2)(n-3)(n-4)(n-5)}\right]\binom{n-2}{s-1}[i^6]_1 + 15\left[\frac{n^2+3n-6sn+6s^2-4}{(n-4)(n-5)}\right]\binom{n-4}{s-2}[i^4]_1[i^2]_1\, N$$

$$+ 10\left[\frac{n^2-n-4sn+4s^2+4}{(n-4)(n-5)}\right]\binom{n-4}{s-2}[i^3]_1^2\, N + 15\binom{n-6}{s-3}[i^2]_1^3\, N^2$$

B.6 Low Values of n

The fourth order moment formulas obviously do not hold for $n = 3$. This results from the use of terms such as $\langle x_i, x_i, x_i, x_i \rangle$ in the expansion of Ave $[\langle x_i \rangle^4]$ and other comparable four subscript summations in the other moments.

Eliminating the contributions of these brackets, and letting $n = 3$ we have

$$[ij^3]_s = \frac{s}{3!} \binom{3}{s} [2 - 7(s-1)] [ij^3]_1$$

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

$$[i^4]_s = \frac{s}{3!} \binom{3}{s} ([2 - 7(s-1)] [i^4]_1 + 3(s-1) N[i^4]_1).$$

Utilizing the results of section 5.3 it is easily shown that these may be written simply as

$$[ij^3]_1 = [ij^3]_2 = 0,$$

$$[i^2j^2]_1 = [i^2j^2]_2 = \frac{N}{6} [i^2]_1 [j^2]_1,$$

$$[i^4]_1 = [i^4]_2 = \frac{N}{2} [i^2]_1^2.$$

Similarly the fifth and sixth order moment formulas do not apply for $n < 5$ and $n < 6$ respectively. However, these formulas were not required for such values of n in this dissertation.