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# APPLICATION OF THE CALCULUS FOR FACTORIAL ARRANGEMENTS: ARBITRARY BLOCK DESIGNS

by Badrig Kurkjian\* Rosalie Woodall

May 1972

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#### ABSTRACT

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A unified method of analysis for factorial arrangements in block designs has been developed for arbitrary block designs. The main results shown here are (1) an easy way to determine the degrees of freedom for treatments, (2) a systematic approach to find a set of estimable effects, and (3) in the factorial case, a method to determine which effects are confounded with blocks or aliased with other effects.

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#### 1. INTRODUCTION

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This report is the fifth effort<sup>1,2,3,4</sup> using a unified method of analysis for factorial argements incorporated into block designs. Four efforts were previously published in various j: mals.<sup>1,2,3,4</sup> The first two papers<sup>1,2</sup> present the basic theory and give solutions for a wide class of balanced (hence connected) block designs. Due to certain desirable properties associated with balanced designs, these solutions can be expressed explicitly and require no inversion of matrices to obtain the solutions. The third<sup>3</sup> treats the case of two-way elimination of heterogeneity. The fourth<sup>4</sup> treats the case involving unequal number of treatments per block but is restricted to the case of designs with one block only and to the case of complete factorial experiments.

This report extends the prior work by providing solutions for arbitrary block designs. Included are nonconnected designs in general, the fractional factorial designs, case of missing treatments in general, and unequal number of treatments per plot per each of multiple blocks. In these cases, the nice properties of balanced designs disappear, and the solutions to the normal equations will sometimes involve matrix inversions for the reduced solutions. Effective use of partitioned matrices, and their generalized inverses, is made in these cases. In many other cases the coefficient matrix of the normal equations is idempotent; then the solution to the reduced normal equations is expressed explicitly without requiring formal matrix inversion.

The main contributions of this paper are: Theorem 1 from which the rank of the coefficient matrix of the reduced normal equations can be determined easily (Section 3.3); a systematic approach to finding the estimable parameters in the non-factorial case for any block design (Sections 3.4 and 3.5); and the extension of the results to the factorial case where the confounded and aliased effect terms are determined in terms of the estimable parameters. (Sections 4.3 and 4.4).

There probably are no new mathematical results herein, although some of the results are hard to find in any one place. The known results used by many authors, notably, Tocher,<sup>5</sup> Rao,<sup>6</sup> Zelen and Goldman,<sup>7</sup> Graybill,<sup>8</sup> Kurkjian and Zelan,<sup>1,2</sup> Kempthorne,<sup>9</sup> are collected together and used to yield a reasonably efficient computer program (FORTRAN IV) to do the analysis. The program requires for input only the observed data and the generalized incidence matrix, L, for the design.

Those designs with especially nice properties, of course, could be solved with more elegant methods.<sup>1,2</sup> Even in these cases, however, a computer program would be desirable for

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Kurkjian, B. and Zelen, M. (1962) A Calculus for Factorial Arrangements Ann. Math. Stot. 33, 609-619.

<sup>&</sup>lt;sup>2</sup>Kurkjian, B. and Zelen, M. (1963) Applications of the Calculus for Factorial Arrangements I. Block and Direct Product Designs, Biometrika <u>50</u>, 63-73.

<sup>&</sup>lt;sup>3</sup>Zelen, M. and Federer, W. T. (1964): Applications of the Calculus for Factorial Arrangements II. Designs with Two-way Elimination of Heterogeneity – Ann. Math. Stat. <u>35</u>, 658-672.

<sup>&</sup>lt;sup>4</sup>Zelen, M. and Federer, W. T. (1966): Application of the Calculus for Factoriul Arrangements III. Analysis of of Factorials with Unequal Numbers of Observations, Sankhya, (A), <u>27</u>, 383-400. <sup>5</sup>Tocher, K. D. (1952) The Design and Analysis of Block Experiments, J. Roy. Stat. Soc., Ser B, <u>14</u>, 45-91.

<sup>&</sup>lt;sup>o</sup>Tocher, K. D. (1952) The Design and Analysis of Block Experiments, J. Roy. Stat. Soc., Ser B, <u>14</u>, 45-91. <sup>6</sup>Rao, C. R. (1962) A Note on a Generalized Inverse of a Matrix With Applications to Problems in Mathematical <sub>2</sub>Statistics. J. Roy Stat. Soc (B), <u>24</u>, 152-158.

<sup>&</sup>lt;sup>7</sup>Zelen, M. and Goldman, A. J. (1954): Weak Ceneralized Inverses and Minimum Variance Linear Unbiased Estimation. J. Res. Nat'l. Bur. Stds. 68B, 151-172.

<sup>&</sup>lt;sup>8</sup>Graybill, F. A. (1961) <u>An Introduction to Linear Statistical Models</u>, Volume I, McGray-Hill, New York. <sup>9</sup>Kempthorne, O. (1952) Design and Analysis of Experiments, John Wiley and Sons, New York.

each type of balanced design to do the unpleasant arithmetic. However, as frequently happens in practice, the balance of a well designed experiment is inadvertently destroyed at the field site through loss of data, or failure to follow the test design for various reasons. In these situations the experimenter need not be concerned with the synthesis and analysis of the resulting of sign. The data are analyzed as taken. The computer output lists the complete analysis of variance together with the estimates of the treatment parameters, the associated parameters of the aliasing and confounding where appropriate.

Following the introduction the paper is divided in 5 parts. Section 2 contains, for completeness, some mathematical tools to be used in the sequel. Section 3 gives a short review for the analysis of block designs to set the stage for 2 e main results given in section 4. An outline of the entire computational procedure is given in section 5. Section 6 gives some examples.

#### 2. MATHEMATICAL TOOLS

T with section we summarize some notation and operations which are used in the sequel.  $\frac{\partial (x, y)}{\partial x} = 0$  (1) in special matrices will be used:

- $x_i$  column vector of dimension m, with all elements unity
- $J_i = 1, 1'_i$  a square matrix of dimension  $m_i$  with all elements unity
- I, the unit matrix of dimension m,
- $\mathbf{M}_{i} = \mathbf{m}_{i} \mathbf{I}_{i} \mathbf{J}_{i}$
- $\mathbf{0}_{i}$  a column vector of dimension  $\mathbf{m}_{i}$  with all null elements

#### 2.1 Direct Product (DP) and Symbolic Direct Product (SDP)

Let  $A = (a_{ij})$  and  $B = (b_{rs})$  be rectangular matrices of dimensions  $m \times n$  and  $p \times q$ , respectively. Then the direct product (DP), or Kronecker product, of A and B will be written  $A \times B$  and is given by

$$A \times B = \begin{bmatrix} a_{11} & B & a_{12} & B & \cdots & a_{\ln} & B \\ a_{21} & B & a_{22} & B & \cdots & a_{2n} & B \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & &$$

with dimensions mp × nq. In general, if  $A_i$ , (i = 1, 2, ..., k), are  $m_i \times n_j$  matrices, their joint direct product,  $A_1 \times A_2 \times ... \times A_k$  will have dimensions

$$\frac{\mathbf{k}}{\prod_{i=1}^{k} \mathbf{m}_{i} \times \prod_{i=1}^{k} \mathbf{n}_{i}}$$

For arbitrary square matrices, A, B, C, and D, the direct product operation has the following basic properties:

$$(\mathbf{A} \times \mathbf{B}) \times \mathbf{C} = \mathbf{A} \times (\mathbf{B} \times \mathbf{C})$$

 $(\mathbf{A} + \mathbf{B}) \times \mathbf{C} = (\mathbf{A} \times \mathbf{C}) + (\mathbf{B} \times \mathbf{C})$ 

 $c \times A = A \times c = cA$  for an arbitrary scalar c

 $(\mathbf{A} \times \mathbf{B})' = \mathbf{A}' \times \mathbf{B}'$ 

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 $(A \times B)^{-1} = A^{-1} \times B^{-1}$  providing the indicated inverses exist

(A  $\times$  B) (C  $\times$  D) = AC  $\times$  BD provided the indicated products are conformable.

The symbolic direct product (SDP) operation will be denoted by  $\otimes$ . Let

 $a'_i = [a_i (1), a_i (2), \cdots, a_i (m_i)]$ 

be row vectors for i = 1, 2, ..., n. Then the SDP of  $a_p$  and  $a_q$  is defined to be

$$a_{p} \otimes a_{q} = \begin{bmatrix} a_{p} & (1) \\ a_{p} & (2) \\ . \\ . \\ . \\ a_{p} & (m_{p}) \end{bmatrix} \otimes \begin{bmatrix} a_{q} & (1) \\ a_{q} & (2) \\ . \\ . \\ . \\ a_{q} & (m_{q}) \end{bmatrix} = \begin{bmatrix} a_{pq} & (1m_{q}) \\ a_{pq} & (1m_{q}) \\ a_{pq} & (21) \\ . \\ . \\ . \\ a_{pq} & (m_{q}) \end{bmatrix}$$

The extension of the SDP to more than two vectors is straightforward. The SDP is an operation on symbolic quantities, but not on numerical quantities.

As an example, let  $m_p = m_q = 2$ . Let  $a_{oq}$  (ij) denote the effect of a two-factor interaction term when experimental factors  $A_p$  and  $A_q$  are at levels i and j, respectively. Then  $a_p \bigotimes a_q$  will be used in the sequel to order the elements of the two factor interaction as

 $[a_{p,q} \otimes a_{q}]' = [a_{p,q} (11) a_{p,q} (12) a_{p,q} (21) a_{p,q} (22)].$ 

Furthermore, the SDP will be used to order the treatment-combinations in a factorial experiment. For example, assume a two-factor experiment with factor A, at two levels and factor A<sub>2</sub> at three levels. Let  $\frac{\partial t_1}{\partial t_1} = (1 \ 2)$  and  $\frac{\partial t_2}{\partial t_2} = (1 \ 2 \ 3)$  be vectors whose elements denote the levels of the factors. Then the SDP

$$\mathcal{C}_1 \otimes \mathcal{C}_2 = \begin{pmatrix} 1 \\ 2 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{bmatrix} 1 & 1 \\ 12 \\ 13 \\ 21 \\ 22 \\ 23 \end{bmatrix}$$

gives the ordering of the six treatment-combinations

#### 2.2 Generalized Inverse (GI)

The generalized inverse has received much attention recently.<sup>6,7,10,11,12,13</sup> It is particularly useful in solving singular linear systems of equations. The GI of an arbitrary matrix C of dimensions  $m \times n$  is denoted by C<sup>+</sup> and is the matrix which satisfies the relations

<sup>&</sup>lt;sup>6</sup>Rao, C. R. (1962) A Note on a Generalized Inverse of a Matrix With Applications to Problems in Mathematical Statistics. J. Roy Stat. Soc (B), <u>24</u>, 152-158. <sup>7</sup>Zelen, M. and Goldman, A. J. (1964): Weak Generalized Inverses and Minimum Variance Linear Unbrased Esti-

mation. J. Res. Nat'l. Bur. Stds. 68B, 151-172.

<sup>&</sup>lt;sup>10</sup>Ben-Israel, A. and Wersay, S. J. (1933), An Elimination Method for Computing the Generalized Inverse of an Arbitrary Complex Matrix, Jour. Assoc. Comp. Mach. <u>10</u>, 532-537.

<sup>11</sup>Grevilla, T. N. E. (1961) The Pseudoinverse of a Rectangular or Singular Matrix and its Application to the Solution of Systems of Linear Equations. SIAM Review, 1, 38-43.

<sup>&</sup>lt;sup>12</sup>Penrose, R. (1955) A Generalized Inverse for Matrices. Proc. Camb. Phil. Soc. <u>51</u>, 405-413.

<sup>&</sup>lt;sup>13</sup>Searle, S. R. (1965) Matrix Algebra for the Biological Sciences, John Wiley and Sons, New York.

The reduced normal equations used here will always be singular, and, hence, the GI will be used to obtain their solution. In many cases, the coefficient matrix C of the normal equations is idempotent, ( $C^2 = C$ ), or quasi-idempotent, ( $C^2 = \lambda C$ ,  $\lambda$  a scalar). In these cases, it is readily verified that the GI of C is given by  $C^* = -\lambda^2$ . For the relatively infrequent cases where C is not quasi-idempotent, the GI is computed using the method of Een-Israel.

#### 3. ANALYSIS OF BLOCK DESIGNS

#### 3.1 Notation and Model

Consider a design involving a fraction or all of v treatments applied to b blocks. Let block j contain  $k_j$  treatments, j = 1, 2, ..., h and let treatment i be replicated  $r_i$ , i = 1, 2, ..., v, times throughout all blocks. For the classical balanced or partially balanced incomplete designs  $k_j$  and  $r_i$  are constants over all i and j. There is no such restriction herein. Furthermore, to introduce unequal number of treatments per plot per block, let  $v_{ij}$  denote the number of times treatment i appears in block j. Hence we will have

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$$r_{i} = \sum_{i=1}^{b} \hat{z}_{ij}.$$

 $k = \sum_{i=1}^{N} i$ 

Let  $y_{ijk}$  denote the yield of the k<sup>th</sup> replication of the i<sup>th</sup> treatment in the j<sup>th</sup> block. We will assume the usual fixed effects model.

$$y_{ijk} = w + t_i + b_j + \epsilon_{ijk}, \quad i = 1, 2, \dots, v$$
  
 $j = 1, 2, \dots, b$  (1)  
 $k = 1, 2, \dots, \epsilon_{ij}$ 

where  $t_i$  is the fixed effect of the i<sup>th</sup> treatment,  $b_j$  the fixed effect of the j<sup>th</sup> block, ... the general effect, and the  $\epsilon_{ijk}$  are independent random variables. (The mixed effects model, using the unified methods herein, has been considered,<sup>14</sup> although it has not been incorporated in this paper.) For the sake of tests of significance it will be assumed that each  $\epsilon_{ijk}$  is distributed normally, N(0,  $c^2$ ). We further assume that effects  $t_i$  and  $b_j$  are subject to the restraints

$$\sum_{i=1}^{v} t_{i} = \sum_{j=1}^{b} v_{j} = 0.$$

<sup>&</sup>lt;sup>14</sup>Kurkjian, B., (1960) General Theory for Asymmetrical, Confounded, Factorial Experiments, TR-829 Harry Diamond Labs., Washington, D.C.

Let  $N = (n_{ij})$  be the  $(v \times b)$  incidence matrix of the design where  $n_{ij} = 0$  or 1 depending on whether the i<sup>th</sup> treatment is absent or present in the j<sup>th</sup> block. Let  $J = (\ell_{ij}) = (n_{ij}, \ell_{ij})$ denote the generalized incidence matrix. Then the least squares estimates of the treatment effects can be obtained in the usual way, by minimizing

$$S = \sum_{i=1}^{v} \sum_{j=1}^{b} \sum_{k=1}^{\ell_{ij}} n_{ij} (y_{ijk} - \mu - t_i - b_j)^2$$

with respect to  $t_i$ ,  $b_j$  and  $\mu$ . Eliminating  $b_j$  and  $\mu$  from the resulting normal equations, one obtains the reduced normal equations, C  $\hat{t} = Q$ , where

$$Q = T - LK^{-1}B$$
,  $C = R - LK^{-1}L'$ 

$$T' = (T_{1} T_{2} \cdot \cdot \cdot T_{V}), \qquad T_{i} = \sum_{j=1}^{b} \sum_{k=1}^{\ell_{ij}} n_{ij} y_{ijk}$$
  

$$B' = (B_{1} B_{2} \cdot \cdot \cdot B_{b}), \qquad B_{j} = \sum_{i=1}^{v} \sum_{k=1}^{\ell_{ij}} n_{ij} y_{ijk} \qquad (2)$$
  

$$R = diag (r_{1} r_{2} \cdot \cdot \cdot r_{v}), \qquad r_{i} = \sum_{j=1}^{b} \ell_{ij}$$
  

$$K = diag (k_{1} k_{2} \cdot \cdot \cdot k_{b}), \qquad k_{j} = \sum_{i=1}^{v} \ell_{ij}$$

The elements of C can be expressed as

$$c_{ii} = r_{i} - \sum_{j=1}^{b} \ell_{ij}^{2} / k_{j}, \quad i = 1, 2, \cdots, v$$

$$c_{is} = -\sum_{j=1}^{b} \ell_{ij} / k_{j}, \quad i, s = 1, 2, \cdots, v, i \neq s$$
(3)

As will be shown in section 3.5 the solution to the reduced normal equations,  $C\hat{t} = Q$ , is given by

$$\hat{t} = C^{\dagger} Q$$
 (4)

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where  $C^+$  is the generalized inverse of C. It can easily be shown, using the expressions (3), that the rows and columns of C sum to zero. Hence the rank of C is always less than v. As will be shown in section 3.3., the concept of connectedness of the design will be useful in determining the rank of C, and, equivalently, the degrees of freedom associated with the treatment sums of squares.

Furthermore it is readily verified that Var  $[Q] = C \sigma^2$  so that the variance-covariance matrix for the treatment effects is given by

Var 
$$(\hat{t}) = C^*$$
 Var  $[O] C^* = C^* \sigma^2$ .

The sums of squares due to treatments can be expressed as

$$SS(t) = \hat{t}' Q = \hat{t}' C \hat{t} = (\hat{t}) [V(\hat{t})]^{\dagger} (\hat{t}) \sigma^{2}.$$

Letting Y =  $(n_{i j} y_{i j k})$  be the vector of observations, w the total number of observations, i.e.,

$$v = \sum_{i=1}^{v} \sum_{j=1}^{b} \ell_{ij}$$

and G the sum of all the observations, i.e.,

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$$G = \sum_{i=1}^{\nu} \sum_{j=1}^{b} \sum_{k=1}^{\ell_{ij}} n_{ij} y_{ijk},$$

the analysis of variance table can be expressed<sup>5,9</sup> as

Source of Variation	Sums of Squares	Degrees of Freedom
Treatments (adjusted for blocks)	t'Q	Rank C
Blocks (unadjusted)	$B'K^{-1}B - G^{2}/w$	b - 1
Error	$Y'Y - \hat{t}'Q - B'K^{-1}B$	w - Rank C - b
Total	$Y'Y - G^2/W$	w - 1

## 3.2 Connected Designs and the Rank of C

A connected design can be defined as follows. Two blocks,  $b_{j_1}$  and  $b_{j_2}$ , are said to be connected if they contain some treatment in common. A third block,  $b_{j_3}$ , is said to be

<sup>&</sup>lt;sup>5</sup>Tocher, K. D. (1952) The Design and Analysis of Block Experiments, J. Roy. Stat. Soc., Ser<u>B</u>, 14, 45-91. <sup>9</sup>Kempthorne, O. (1952) <u>Design and Analysis of Experiments</u>, John Wiley and Sons, New York.

connected to both of these blocks, if it has at least one treatment in common with either of the blocks  $b_{j_1}$  or  $b_{j_2}$ . All blocks connected in such a manner are said to form a set of connected blocks. If all blocks in a given design, involving all v treatments, are connected through such a chein of common treatments, the design is said to be connected and to consist of one set of connected blocks,  $S = (b_1, b_2, \ldots, b_b)$  where elements of S denote the block labels.

For connected designs with no missing treatments it is well known<sup>5</sup> that the rank of C is v - 1. That is, for connected designs it is readily shown that one can construct (v - 1) linearly independent relationships between the treatment parameters. Hence the rank of C is v - 1. Consequently, the one constraint

$$\sum_{i=1}^{\nu} t_i = 0,$$

inherent in the model, is all that is required to get a unique solution to the reduced normal equations  $C\hat{t} = Q$ .

Using the calculus for factorial arrangements, the analysis of balanced (hence connected) incomplete block designs is particularly elegant and simple<sup>1.2</sup>. The main purpose of this paper is to extend the basic results of Kurkjian and Zelen to the case of disconnected designs.

#### 3.3 Disconnected Designs, Missing Treatments, and the Rank of C

When all the blocks are not connected via a chain of common treatments, the design is said to be disconnected. In this case there will be more than one set of connected blocks. For example, the design with incidence matrix

$$N = \left( \begin{array}{ccc} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right)$$

is disconnected since block 2 has no treatment in common with blocks 1 and 3. Since blocks 1 and 3 are connected via treatment 1, the design N is said to decompose into two sets of connected blocks:  $S_1 = (b_1, b_3)$  and  $S_2 = (b_2)$ .

In general, the determination of the number of sets,  $z_1$ , of connected blocks is a trivial task, obtained by inspection of the incidence matrix of the design.

As the following theorem shows, the number of distinct sets of connected blocks,  $z_1$ , and the number of missing treatments,  $z_2$ , in the design will determine the rank of the coefficient

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<sup>&</sup>lt;sup>1</sup>Kurkjian, B. and Zelen, M. (1962) A Calculus for Factorial Arrangements Ann. Math. Stat. <u>33,</u> 609-619.

<sup>&</sup>lt;sup>2</sup>Kurkjian, B. and Zelen, M. (1963) Applications of the Calculus for Factorial Arrangements I. Block and Direct Product Designs, Biometrika 50, 63-73.

<sup>&</sup>lt;sup>5</sup>Tocher, K. D. (1952) The Design and Analysis of Block Experiments, J. Roy. Stat. Soc., Ser B, <u>14</u>, 45-91.

matrix C of the reduced normal equations and, hence, the total number of constraints required to achieve a unique solution to these equations. Moreover, rank C also yields the degrees of freedom associated with the treatment sums of squares in the analysis of variance table.

Theorem 1. For any block design, the rank of the  $v \times v$  coefficient matrix C of the reduced normal equations  $C\hat{t} = Q$ , is  $v - z_1 - z_2$ , where v is the total number of treatments in the experiment,  $z_1$  is the number of sets of connected blocks, and  $z_2$  is the number of treatments for which no observations were taken during the experiment.

Proof: Without loss of generality, one may assume that the first  $q_1$  treatments are associated with the first set of  $p_1$  connected blocks, the second  $q_2$  treatments with the second set of  $p_2$  connected blocks, and the penultimate  $q_{z_1}$  treatments with the  $z_1^{th}$  set of  $p_{z_1}$  connected blocks. Moreover, let the last  $z_2$  treatments be those missing in the experiment. This assignment could be achieved through appropriate relabeling of treatments and blocks. With such a rearrangement, it follows directly from the definition of connected blocks, that the generalized incidence matrix L can be written in partitioned form as:

$$\mathbf{L} = \begin{bmatrix} \mathbf{L}_{1} (\mathbf{q}_{1} \times \mathbf{p}_{1}) & 0 (\mathbf{q}_{1} \times \mathbf{p}_{2}) \cdots & 0 (\mathbf{q}_{1} \times \mathbf{p}_{z_{1}}) \\ 0 (\mathbf{q}_{2} \times \mathbf{p}_{1}) & \mathbf{L}_{2} (\mathbf{q}_{2} \times \mathbf{p}_{2}) \cdots & 0 (\mathbf{q}_{2} \times \mathbf{p}_{z_{1}}) \\ \vdots & \vdots & \ddots & \vdots \\ 0 (\mathbf{q}_{z_{1}} \times \mathbf{p}_{1}) & 0 (\mathbf{q}_{z_{1}} \times \mathbf{p}_{2}) \cdots & \mathbf{L}_{z_{1}} (\mathbf{q}_{z_{1}} \times \mathbf{p}_{z_{1}}) \\ 0 (\mathbf{z}_{2} \times \mathbf{p}_{1}) & 0 (\mathbf{z}_{2} \times \mathbf{p}_{2}) \cdots & 0 (\mathbf{z}_{2} \times \mathbf{p}_{z_{1}}) \end{bmatrix}$$

where the dimensions of each of the eleme de of L is given in the parenthesis. Clearly then,

$$v = \sum_{i=1}^{z_1} q_i + z_2$$

and the  $(v \times v)$  coefficient matrix,  $C = R - LK^{-1}L'$ , can be written in partitioned form as the diagonal matrix:

$$C = diag [C_1 (q_1 \times q_1) C_2 (q_2 \times q_2) \cdot \cdot C_{z_1} (q_{z_1} \times q_{z_1}) 0 (z_2 \times z_2)]$$

In accordance with section 3.2, the rank of each  $C_k$ , k = 1, 2, ...,  $z_1$ , is  $(q_k - 1)$ , since each partition is associated with a set of connected blocks. Hence, it follows that

Rank C = 
$$\sum_{k=1}^{z_1} (q_k - 1) = v - z_2 - z_1$$
.

which completes the proof.

Since v,  $z_1$ , and  $z_2$  are obtained almost instantly by inspection of the incidence matrix of any arbitrary block design, the number of estimable treatment parameters and, hence, the degrees of freedom associated with the treatment sums of squares is reduced to the trivial calculation  $v - z_1 - z_2$ .

#### 3.4 Choice of Constraint Matrix

To achieve a unique solution to the normal equations,  $\hat{Ct} = Q$ , where rank  $C = v - z_1 - z_2$ , we will need  $(z_1 + z_2)$  additional independent relationships between the treatment effects. In this paper we obtain these relationships by adopting the convention that the sum of the treatment effects associated with each set of connected blocks is zero, i.e., each treatment parameter is expressed about the mean of the effects associated with that particular set of connected blocks. Moreover, for each missing treatment in the design, the corresponding treatment effect will be assumed expressed about its own true value, hence, assigned the value zero.

This convention is quite commonly used by other investigators although it may not be explicitly stated in their published works.

With the treatment labeling as given in theorem 1, this convention can be expressed mathematically as the solution to U' $\hat{t} = 0$  where U' is the  $[(z_1 + z_2) \times v]$  matrix

$$U' = \operatorname{diag} \left( 1_{q_1}' 1_{q_2}' \cdots 1_{q_{z_1}}' I_{z_2} \right)$$
 (5)

It follows immediately from the proof of theorem 1 and from the fact that the rows and columns of C sum to zero, that U'C = 0. Moreover, it is obvious that

$$\det (U' U) = \prod_{i=1}^{s_1} q_i$$

and, hence, is not zero. In general, U' can be written on inspection of L.

#### 3.5 Estimation for Block Designs

For the constraint matrix U', with properties U'C = 0 and det  $(U'U) \neq 0$ , the solutions to the augmented normal equations

$$\begin{pmatrix} C & U \\ U' & 0 \end{pmatrix} \begin{pmatrix} t \\ 0 \end{pmatrix} = \begin{pmatrix} Q \\ 0 \end{pmatrix}$$
(6)

can be shown to be<sup>7</sup>

<sup>&</sup>lt;sup>7</sup>Zelen, M. and Goldman, A. J. (1964): Weak Generalized Inverses and Minimum Variance Linear Unbiased Estimation. J. Res. Nat<sup>1</sup>I. Bur. Stds. 68B, 151-172.

## $\hat{\mathbf{t}} = \mathbf{C}^{\dagger} \mathbf{Q},$

where  $C^*$  is the GI of C. Fortunately, for many designs, C has the property that  $C^2 = \lambda C$ where  $\lambda$  is a scalar constant. In such cases the GI of C is readily verified to be  $C^* = C/\lambda^2$ . The digital program developed for this analysic checks the coefficient matrix C for this idempotency property at the outset. When C is not idempotent, then the GI is computed using the method of Ben-Israel and Wersay.<sup>10</sup>

The results of section 3 are sufficient for the analysis of experiments involving simple treatments applied to any arbitrary block design, balanced, connected, or not. The next section extends the results to the case of experiments involving factorial treatment-combinations applied to general block designs.

#### 4. ANALYSIS OF FACTORIAL EXPERIMENTS IN BLOCK DESIGNS

#### 4.1 Notation and Model

Consider now a factorial experiment involving n experimental factors,  $A_s$ , where factor  $A_s$  appears at  $m_s$  levels,  $s = 1, 2, \ldots, n$ . A particular selection of levels for each factor,  $i = (i_1 \ i_2 \ \ldots \ i_n)$ , will be termed the i<sup>th</sup> treatment-combination,  $i = 1, 2, \ldots, v$ , where

$$v = \prod_{n=1}^{n} m_s.$$

Let  $\theta'_s = (1, 2, \ldots, m_s)$  be a vector whose elements denote the levels at which factor  $A_s$  appears. Then the SDP,  $\theta_1 \oplus \theta_2 \oplus \ldots \oplus \theta_n$ , a column vector of dimension v, will be used to label and order the v different treatment-combinations. For example for two factors each at two levels, we have the vector of four treatment-combinations given by

$$\theta_1 \otimes \theta_2 = \begin{pmatrix} 1 \\ 2 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{bmatrix} 11 \\ 12 \\ 21 \\ 22 \end{bmatrix}$$

Hence treatment 1 is composed of the first levels of each of the two factors  $A_1$  and  $A_2$ , etc. Treatment i is the element in the i<sup>th</sup> row of  $\theta_1 \odot \theta_2$ , i = 1, 2, 3, 4.

These treatments then are applied to any block design to estimate the effects of the experimental factors acting alone or in interaction with other factors. For this purpose let  $a'_s = (a_s(i_s))$  denote a row vector of length  $m_s$  whose general element  $a_s(i_s)$  represents the effect of the experimental factor  $A_s$  at level  $i_s$ . Moreover, let  $a_{rs}(i_r, i_s)$  denote the effect of the two factor interaction associated with factors  $A_r$  and  $A_s$  at levels  $i_r$  and  $i_s$ , respectively.

(7)

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<sup>&</sup>lt;sup>10</sup>Ben-Israel, A. and Wersay, S. J. (1963), An Elimination Method for Computing the Generalized Inverse of an Arbitrary Complex Matrix, Jour. Assoc. Comp. Mach. <u>10</u>, 532-537.

Then the vector

$$[a_r \otimes a_s]' = [a_{rs}(11), a_{rs}(12), \cdots a_{rs}(1m), a_{rs}(21), \cdots a_{rs}(2m), \cdots$$

$$a_{rs} (m_r 1), \cdots a_{rs} (m_r m_s)$$

displays the  $m_r m_s$  two-factor interaction parameters associated with the experimental factors  $A_r$  and  $A_s$ .<sup>1,2</sup> Likewise,  $\begin{bmatrix} a_{i_1} \otimes a_{i_2} \\ & & \\ & & \\ & & \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} a_{i_p} \end{bmatrix}$  is a row vector displaying the

$$p$$
  
 $j=1$   $m_{i_j}$ 

interaction parameters associated with the p factor interaction  $A_{i_1}$ ,  $A_{i_2}$ ,  $A_{i_p}$ . Clearly, there will be  $2^n - 1$  vectors containing

$$\frac{n}{\left| \frac{1}{1+1} \right|} (1+m_i) - 1$$

such parameters in all. It is quite common in practice<sup>15</sup> to express the treatment effects,  $\mathbf{t}_{i}$  , in terms of these main effect and interaction parameters as

$$t_{i} = \sum_{s=1}^{n} a_{s}(i_{s}) + \sum_{1 \le s} \sum_{r \le n} a_{rs}(i_{r}, i_{s}) + \dots + a_{12, \dots n}(i_{1}, i_{2}, \dots i_{n}),$$
(8)

$$i = 1, 2, \ldots v$$

These relations can be written<sup>1</sup> in matrix form as

$$t = \sum_{k=1}^{n} \sum_{a_{1}+\ldots+a_{n}=k} \{a_{1}((a_{1})) * a_{2}((a_{2})) * \ldots * a_{n}((a_{n}))\}$$
(9)

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Kurkjian, B. and Zelen, M. (1962) A Calculus for Factorial Arrangements Ann. Math. Stat. 33, 609-619.

<sup>&</sup>lt;sup>2</sup>Kurkjian, B. And Zelen, M. (1963) Applications of the Calculus for Factorial Arrangements I. Block and Direct Product Designs, Biometrika <u>50</u>, 63-73. <sup>15</sup>Zelen, M. (1958) The Use of Group Divisible Designs for Confounded Asymmetrical Foctorial Arrangements, Ann

Math Stat. 29, 22-40.

where

$$\mathbf{a}_{i}((\alpha_{i})) = \begin{cases} \mathbf{a}_{i} & \text{if } \alpha_{i} = 1\\ 1_{i} & \text{if } \alpha_{i} = 0 \end{cases}$$
$$\mathbf{a}_{i}((\alpha_{i})) * \mathbf{a}_{j}((\alpha_{j})) = \begin{cases} \mathbf{a}_{i} \otimes \mathbf{a}_{j} & \text{if } \alpha_{i} = \alpha_{j} = 1\\ \mathbf{a}_{i} \times 1_{j} & \text{if } \alpha_{i} = 1, \ \alpha_{j} = 0\\ 1_{i} \times \mathbf{a}_{j} & \text{if } \alpha_{i} = 0, \ \alpha_{j} = 1\\ 1_{i} \times 1_{j} & \text{if } \alpha_{i} = \alpha_{j} = 0. \end{cases}$$

In the starred operations in eq. (9) the products  $a_i \times a_j$  and  $a_i \otimes 1_j$  are not defined and arc termed inadmissible products.

When admissible direct and symbolic direct products both appear in eq. (9), we adopt the convention that DP's are formed first and followed by the SDP's. For example if n = 3,  $m_1 = m_2 = m_3 = 2$ ,  $\alpha_1 = \alpha_3 = 1$ ,  $\alpha_2 = 0$ , we have

$$a_1((a_1)) * a_2((a_2)) * a_3((a_3)) = (a_1 \times 1_2) \otimes a_3$$

$$= \begin{pmatrix} a_{1} (1) \\ a_{1} (2) \end{pmatrix} \times \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} a_{3} (1) \\ a_{3} (2) \end{pmatrix} = \begin{pmatrix} a_{1} (1) \\ a_{1} (1) \\ a_{1} (2) \\ a_{1} (2) \end{pmatrix} \otimes \begin{pmatrix} a_{3} (1) \\ a_{3} (2) \end{pmatrix}$$

 $\begin{bmatrix} a_{13} (11) \\ a_{13} (12) \\ a_{13} (11) \\ a_{13} (12) \\ a_{13} (12) \\ a_{13} (21) \\ a_{13} (22) \\ a_{13} (21) \\ a_{13} (22) \end{bmatrix}$ 

It is easy to verify that this operation is associative. These interaction parameters are no. linearly independent and are taken to satisfy the linear relationship that, for any set of  $m_{FIR}$  effect or interaction terms, the sum over the levels of any single factor is zero. In matrix

form these constraints can be written<sup>1</sup>

$$1'_{s}a_{s} = 0$$
  $s = 1, 2, ..., n$ 

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$$\begin{pmatrix} \mathbf{1}_{\mathbf{r}}^{\prime} \times \mathbf{I}_{\mathbf{s}} \\ \mathbf{I}_{\mathbf{r}} \times \mathbf{1}_{\mathbf{s}}^{\prime} \end{pmatrix} \qquad [\mathbf{a}_{\mathbf{r}} \otimes \mathbf{a}_{\mathbf{s}}] = \begin{pmatrix} \mathbf{0}_{\mathbf{s}} \\ \mathbf{0}_{\mathbf{r}} \end{pmatrix} \mathbf{r}, \ \mathbf{s} = \mathbf{1}, \ \mathbf{2}, \dots, \mathbf{n} \\ \mathbf{r} < \mathbf{s} \\ \vdots \\ \mathbf{0}_{\mathbf{r}} \end{pmatrix} \mathbf{r} < \mathbf{s}$$

$$\vdots \\ \mathbf{1}_{\mathbf{1}}^{\prime} \times \mathbf{I}_{\mathbf{2}}^{\prime} \times \dots \times \mathbf{I}_{\mathbf{n}} \\ \mathbf{I}_{\mathbf{1}} \times \mathbf{1}_{\mathbf{2}}^{\prime} \times \dots \times \mathbf{I}_{\mathbf{n}} \\ \mathbf{I}_{\mathbf{1}} \times \mathbf{I}_{\mathbf{2}}^{\prime} \times \dots \times \mathbf{I}_{\mathbf{n}} \end{pmatrix} [\mathbf{a}_{\mathbf{1}} \otimes \mathbf{a}_{\mathbf{2}} \otimes \dots \otimes \mathbf{a}_{\mathbf{n}}] = \begin{pmatrix} \mathbf{0}_{\mathbf{2}} \times \mathbf{0}_{\mathbf{3}} \times \dots \times \mathbf{0}_{\mathbf{n}} \\ \mathbf{0}_{\mathbf{1}} \times \mathbf{0}_{\mathbf{3}} \times \dots \times \mathbf{0}_{\mathbf{n}} \\ \vdots \\ \mathbf{0}_{\mathbf{1}} \times \mathbf{0}_{\mathbf{2}} \times \dots \times \mathbf{0}_{\mathbf{n}} \\ \mathbf{0}_{\mathbf{1}} \times \mathbf{0}_{\mathbf{2}} \times \dots \times \mathbf{0}_{\mathbf{n}-\mathbf{1}} \end{pmatrix}$$

$$(10)$$

It is easy to show that for connected designs with no missing treatments (z  $_1 = 1$ , z $_2 = 0$ ) there will result

$$\sum_{s=1}^{n} (m_{s}-1) + \sum_{r \leq s} (m_{r}-1) (m_{s}-1) + \cdots + \prod_{i=1}^{n} (m_{i}-1) = v - 1$$

linearly independent interaction parameters. Also, it is well known (section 4.2) that these (v-1) linearly independent parameters are expressable as linear combinations of the elements of  $\hat{t}$  which are obtained from the reduced normal equations  $\hat{Ct} = Q$ . For the case where  $z_1 + z_2 > 1$ , the further constraints U' $\hat{t} = 0$  on the  $\hat{t}$  parameters will also have to be imposed on the (v-1) interaction parameters.

<sup>1</sup>Kurkjian, B. and Zelen, M. (1962) A Calculus for Factorial Arrangements Ann. Math. Stat. <u>33</u>, 609-619.

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#### 4.2 Estimation for the Factorial Case for Connected Designs and No Missing Treatments

This case has been treated fully <sup>1,2</sup> using the basic method of this paper. The main results are restated here for completeness and to set the stage for some results in section 4.3 below. Let  $X = (x_1 x_2 \dots x_n)$  be a vector representing an interaction term where the element  $x_i$  is defined as

$$x_i = 1$$
 if factor  $A_i$  is present in the interaction X  
 $x_i = 0$  if factor  $A_i$  is absent in the interaction,  
(11)

Clearly, there will be  $2^n - 1$  such vectors. The vector  $X = (0 \dots 010 \dots 0)$  with a one in the r<sup>th</sup> position and all other elements zero denotes the main effect of factor  $A_r, x = (0 \dots 010 \dots 010 \dots 010 \dots 010 \dots 010 \dots 0)$  with elements in the r<sup>th</sup> and s<sup>th</sup> positions equal to one and all others zero, denotes the two-factor interaction  $A_rA_s$ , etc.,  $X = (11 \dots 1)$  with all elements unity denoting the n-factor interaction  $A_1A_2 \dots A_n$ . For the purposes of this paper, the vectors  $X_i$ ,  $i = 1, 2, \dots, 2^n - 1$  will be ordered as follows: All vectors denoting main effect terms first, those denoting two-factor interaction second, etc., with the n-factor interaction term last. Within each of these groups, (i.e., interaction terms) the vectors are ordered lexicographically. For example, if n = 3, we will have  $2^3 - 1 = 7$  vectors in the following order: (100), (010), (001), (110), (101), (011), (111).

Now let

$$a(X) = a_1^{x_1} \otimes a_2^{x_2} \otimes \ldots \otimes a_n^{x_n}, \sum_{i=1}^n x_i = p$$
 (12)

denote the effect of a particular p-factor interaction term where  $a_i^{x_i} = a_i$  if  $x_i = 1$  and where  $a_i$  is suppressed on the right-hand-side of eq. (12) if  $x_i = 0$ .

As shown by Kurkjian and Zelen,<sup>1</sup> the minimum variance unbiased estimator for a(X) is given by

$$\hat{a}(X) = M(X) \hat{t}/v = M(X) C^{+} Q/v$$
 (13)

where

$$M_{i}^{x_{i}} = M_{i}^{x_{1}} \times M_{2}^{x_{2}} \times \ldots \times M_{n}^{x_{n}}$$
$$M_{i}^{x_{i}} = M_{i} = m_{i} I_{i} - J_{i} \quad \text{if } x_{i} = 1$$
$$= 1; \qquad \text{if } x_{i} = 0$$

<sup>&</sup>lt;sup>1</sup>Kurkjian, B. and Zelen, M. (1962) A Calculus for Factorial Arrangements Ann. Math. Stat. <u>33</u>, 609-619.

<sup>&</sup>lt;sup>2</sup>Kurkjian, B. and Zelen, M. (1963) Applications of the Calculus for Factorial Arrangements I. Block and Direct Product Designs, Biometrika <u>59</u>, 63-73.

Moreover, it follows directly that

Var 
$$[\ddot{a}(X)] = M(X) C^{*} M(X) \sigma^{2} / v^{2} = \Sigma(X) \sigma^{2}$$
, where  
(14)  
 $\Sigma(X) = M(X) C^{*} M(X) r / v^{2}$ 

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Likewise, for different interaction terms  $X_i$  and  $X_i$ ,

Cov 
$$[\hat{a}(X_i), \hat{a}(X_i)] = M(X_i) C^{\dagger} M(X_i)' \sigma^2/v^2.$$
 (15)

Using a result given by  $\operatorname{Rao}^6$  and Zelen and Goldman,<sup>7</sup> the sums of squares associated with the interaction term X is given by

SS 
$$(a(X)) = \hat{a}'(X) [Var \hat{a}(X)]^{\dagger} \hat{a}(X) \sigma^2 = \hat{a}'(X) \Sigma(X)^{\dagger} \hat{a}(X).$$
 (16)

Under the null hypothesis of no interaction effect, SS(a(X)) is distributed as a chi-square variate with degrees of freedom equal to the rank of Var  $[\hat{a}(X)]$ .

If the design is orthogonal (i.e., Cov  $[a(X_i), a(X_j)] = 0$  for all i, j,  $i \neq j$ ), then it is known that

SS (t) = 
$$\hat{t}' Q = \sum_{i=1}^{2^{n}-1} SS[a(X_i)].$$
 (17)

If the design is not orthogonal then the  $SS(a(X_i))$  are not additive. However, as shown by Graybill,<sup>5</sup> each quadratic form,  $SS(a(X_i))$ , is statistically independent of the error sum of squares. Hence, tests of significance based on the F distribution are still valid.

The analysis of variance table is given by

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<sup>&</sup>lt;sup>6</sup>Rao. C. R. (1962) A Note on a Generalized Inverse of a Matrix With Applications to Problems in Mathematical Statistics. J. Roy Stat. Soc (B), <u>24</u>, 152-158.

<sup>&</sup>lt;sup>3</sup>Zelen, M. and Goldman, A. J. (1964) Weak Generalized Inverses and Minimum Variance Linear Unbiased Estimation. J. Res. Nat'l. Bur. Stds. <u>68B</u>, 151-172.

<sup>&</sup>lt;sup>8</sup>Graybill, F. A. (1961) <u>An Introduction to Linear Statistical Models</u>, Volume 1, McGray-Hill, New York.

Source of Variation	Sums of Squares	Degrees of Freedom
$\mathbf{x}_1$	$SS(a(X_1))$	Rank $\Sigma(X_1)$
X <sub>2</sub>	SS(a(X <sub>2</sub> ))	Rank $\Sigma(X_2)$
•	•	
•	•	
•	•	
$X_{2^{n}-1}$	$SS(a(X_{2^{n-1}}))$	Rank $\Sigma(X_{2^{n}-1})$
Blocks (unadjusted)	$B'K^{-1}B - G^2/w$	b - 1
Error	$Y'Y - \hat{t}Q - B'K^{-1}B$	w - Rank C - b
Total	$Y'Y - G^2/W$	w - 1

# 4.3 Estimation for the Factorial Case for Disconnected Designs with Missing Treatments $(z_1 + z_2 > 1)$

As indicated in section 3.3, for the general case when the design is not connected or only a fraction of the treatment-combinations are tested, the rank of the coefficient matrix, C, of the reduced normal equations is  $v-z_1-z_2$ . In this case one must select a particular set of  $v-z_1-z_2$  parameters for which a unique solution to the normal equations will exist. In this paper the selection is made as follows. First eliminate those parameters that are dependent as a consequence of the basic constraints (eq. 10). This is done by eliminating all but the  $(m_i - 1)$  lowest level parameters of the main effect vectors,  $a(X_i)$ , associated with the experimental factors  $A_i$ ,  $i = 1, 2, \ldots$ , n; all but the  $(m_i - 1)$   $(m_j - 1)$  lowest level parameters of the two-factor interaction vectors associated with experimental factors  $A_i A_j, \ldots$ ; and all but the

$$\prod_{i=1}^{n} (m_i - 1)$$

lowest level parameters belonging to the n-factor interaction  $A_1 A_2 \ldots A_n$ . Hence, all but (v-1) parameters are eliminated. Second,  $(z_1 + z_2 - 1)$  of these v - 1 parameters must be eliminated because they can be expressed as linear functions of the remaining  $(v - z_1 - z_2)$  parameters through the relationships resulting from the constraint equation  $U'\hat{t} = 0$  of section 3.4. One chooses the  $(z_1 + z_2 - 1)$  parameters to be those which are unestimable (as defined in section 4.3 below) or those associated with higher order interaction terms.

To clarify this parameter selection scheme, and to set the stage for an efficient computational algorithm for the estimation problem, it is convenient to introduce the following quantities.

Let a denote the universal vector, of dimension

$$\frac{n}{1}$$
 (1 + m<sub>i</sub>) - 1,

containing all the main and interaction effect parameters,

$$a' = [a'(X_1) - a'(X_2) + ... a'(X_{2^{n-1}})],$$
 (18)

where the interaction vectors,  $X_i$ , are ordered as indicated in section 4.2. Similarly, let M, of dimension

$$\frac{n}{1+1} (1 + m_i) - 1 \times v,$$

be a matrix made up of the corresponding  $M(X_i)$  matrices, i.e.

$$M' = [M'(X_1) \qquad M'(X_2) \ldots M'(X_{2^{n-1}})].$$

Now let  $\overline{a}$  denote the vector of v - 1 elements remaining after elimination of the parameters that are dependent because of the basic constraints of eq. (10), and let  $\overline{M}$  be the matrix consisting of the corresponding rcws of M. Thus, we have for reference

$$\overline{\mathbf{a}}' = \left[\overline{\mathbf{a}} (X_1) \quad \overline{\mathbf{a}}'(X_2) \ldots \overline{\mathbf{a}}' (X_{2^{n-1}})\right],$$

and

$$\overline{\mathbf{M}}' = [\overline{\mathbf{M}}'(\mathbf{X}_1) \qquad \overline{\mathbf{M}}'(\mathbf{X}_2) \cdots \overline{\mathbf{M}}'(\mathbf{X}_{n-1})].$$

Let  $\overline{\overline{a}}' = [\overline{\overline{a}}' (X_{i_1}) \ \overline{\overline{a}}' (X_{i_2}) \dots \overline{\overline{a}}' (X_{i_1})]$  denote the vector containing a total of  $v - z_1 - z_2$  parameters that remain after the further elimination of parameters in  $\overline{a}$ , through application of the constraint equation

$$U't = U'\sum_{s=1}^{n}\sum_{\sum a_{i}=s} a_{1}^{a_{1}} * a_{2}^{a_{2}} * \dots * a_{n}^{a_{n}} = 0.$$
(19)

Removing the cor. sponding rows of M there results

$$\overline{\overline{\mathbf{M}}}' = \left[\overline{\overline{\mathbf{M}}}' \quad \left( \cdot_{\mathbf{i}_{1}} \right) \qquad \overline{\overline{\mathbf{M}}}' \left( \mathbf{X}_{\mathbf{i}_{2}} \right) \cdots \overline{\mathbf{M}}' \quad \left( \mathbf{X}_{\mathbf{i}_{s}} \right) \right]$$

The vector  $\overline{a}$  now contains the  $v - z_1 - z_2$  linearly independent parameters which permit unbiased minimum variance estimation and, hence, are termed estimable parameters in the standard sense.<sup>8</sup> In this paper elements of  $\overline{a}$  will be termed independent parameters. Elements

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<sup>&</sup>lt;sup>8</sup>Graybill, F. A. (1961) <u>An Introduction to Linear Statistical Models</u>, Volume I, McGray-Hill, New York.

of a that do not appear in  $\overline{\overline{a}}$  will be termed dependent parameters. The interaction  $X_i$ ,  $j = 1, 2, \ldots$ , s, is represented in  $\overline{\overline{a}}$  if at least one element of  $a(X_i)$  is a member of  $\overline{\overline{a}}$ . Such interactions will be termed estimable or unestimable in the sense described in the next section. The original singular system of normal equations has now been reduced to a non-singular system of rank  $C = v - z_1 - z_2$  and, hence, yields the following standard quantities as solutions.

$$\overline{\overline{a}} \left( X_{i_{j_{j_{j_{j}}}}} \right) = \overline{\overline{M}} \left( X_{i_{j_{j_{j}}}} \right) \widehat{t} / v = \overline{\overline{M}} \left( X_{i_{j_{j}}} \right) C^{*} O / v$$

$$V_{\text{far}} \left( \overline{\overline{a}} \left( X_{i_{j_{j}}} \right) \right) = \overline{\overline{M}} \left( X_{i_{j_{j}}} \right) C^{*} \overline{\overline{M}}' \left( X_{i_{j_{j}}} \right) \sigma^{2} / v^{2} = \sigma^{2} \overline{\Sigma} \left( X_{i_{j_{j}}} \right)$$

$$Cov \left( \overline{\overline{a}} \left( X_{i_{j_{j_{j}}}} \right) \overline{\overline{a}} \left( X_{i_{j_{2}}} \right) \right) = \overline{\overline{M}} \left( X_{i_{j_{2}}} \right) C^{*} \overline{\overline{M}}' \left( X_{i_{j_{2}}} \right) \sigma^{2} / v^{2}, \ j_{1} \neq j_{2}$$

$$SS \left( a(X_{i_{j}}) \right) = \overline{\overline{a}}' \left( X_{i_{j_{j}}} \right) \overline{\Sigma} \left( X_{i_{j_{j}}} \right)^{-1} \overline{\overline{a}} \left( X_{i_{j_{j}}} \right)$$

$$i = 1, 2, \dots, S$$

$$(20)$$

The analysis of variance table is given by:

AND DESCRIPTION OF

Source of Variation	Sums of Squares	Degrees of Freedom
X <sub>i</sub>	SS(a(X <sub>i</sub> ))	Rank $\overline{\overline{\Sigma}}$ (X <sub>i</sub> )
X <sub>i</sub>	SS(a(X, 2))	$\mathbf{Rank} = (\mathbf{X}_{i_{2}})$
•		•
•	•	•
•	•	•
Blocks (unadjusted)	$BK^{-1}B - G^2/w$	b - 1
Error	$\mathbf{Y}' \mathbf{Y} - \mathbf{\hat{t}}' \mathbf{Q} - \mathbf{B}' \mathbf{K}^{-1} \mathbf{B}$	w - Rank C - b
Total	Y'Y - G <sup>2</sup> /w	w - 1

#### 4.4 Unestimable, Aliased, and Confounded Interactions

The theory of confounding and aliasing is easy to apply for the case of  $2^n$  designs. However for general designs the determination of such effects is quite difficult. The literature in many cases identifies the aliased and confounded interactions without giving the mathematical foundation for the determination. In this paper the definition of such effects is based on the linearly independent, hence estimable, parameters in the solution to the normal equations, i.e. the elements of a in section 4.3

Consider an effect vector  $a(X_{\beta})$  associated with the interaction  $X_{\beta}$ ,  $\beta = 1, 2, ..., 2^n - 1$ . The following definitions will be used to characterize its estimability.

### Definition 1. Estimable and Unestimable Interactions

If all elements of  $a(X_{\beta})$  belonging to  $\overline{a}$  are also in  $\overline{a}$ , the interaction  $X_{\beta}$  is termed estimable. If some (or all) of the elements of  $\overline{a}(X_{\beta})$  do not belong to  $\overline{\overline{a}}$ , then the interaction  $X_{\beta}$  is said to be partially (or totally) unestimable. Some unestimable interactions can further be classified as aliased or confounded.

#### Definition 2. Aliased Interactions

An interaction  $X_{\beta}$  will be termed an alias of a lower order, at least partially estimable interaction  $X_{\alpha}$ , if at least one dependent effect parameter associated with  $X_{\beta}$  is linearly dependent on at least one independent effect parameter associated with  $X_{\alpha}$ . It should be noted that this definition allows partially unestimable interactions to be aliased with more than one lower order interaction.

#### Definition 3. Confounded Interactions

If for the interaction  $X_{\beta}$ :

- (i) the effect vector  $a(X_{\beta})$  contains only dependent parameters, i.e., has no elements in  $\overline{a}$ , and
- (ii) each of these dependent parameters is not linearly related to any of the independent elements in a, and
- (iii) b > 1,

then  $X_{\beta}$  is said to be completely confounded with blocks. If b = 1, then  $X_{\beta}$  is said to be completely unestimable.

## Definition 4. Partially Confounded (Unestimable) Interactions

If the effect vector  $\overline{a}(X_{\beta})$  associated with the interaction  $X_{\beta}$  contains dependent elements that are linearly related only to its own independent elements, then  $X_{\beta}$  is said to be partially confounded with blocks, provided b > 1. If b = 1,  $X_{\beta}$  is said to be partially unestimable.

## 5. COMPUTATIONAL PROCEDURE

The computational procedure can be summarized as follows:

<u>Step 1.</u> Given the generalized incidence matrix L and the vector of observations,  $Y = (n_{ij} y_{ijk})$ , compute C and Q (cf. section 3.1).

Step 2. Compute the generalized inverse C<sup>+</sup> and obtain the solution to the reduced normal equations, i.e.  $\hat{t} = C^+Q$  (cf. section 3.5).

Step 3. By inspection of L determine  $z_1$  and  $z_2$  and compute rank  $C = v - z_1 - z_2$  (cf. section 3.3).

Step 4. Compute the analysis of variance table as indicated in section 3.1.

For factorial experiments, the following additional computations are made. The treatment combinations and the rows of L must be labeled and ordered in accordance with section 4.1.

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Step 5. Compute the main and interaction effect vectors  $\hat{a}(X_i) = M(X_i) \hat{t}/v$  and form  $\overline{\hat{a}}(X_i)$  and  $\overline{M}(X_i)$ ,  $i = 1, 2, ..., 2^n - 1$  (cf. section 4.2). If rank C = v - 1, set  $\overline{\hat{a}}(X_i) = \overline{\hat{a}}(X_i)$  and  $\overline{M}(X_i) = \overline{M}(X_i)$ , and proceed to step 9.

<u>Step 6.</u> Construct, by inspection (cf. section 3.4) the constraint matrix U', of dimension  $(z_1 + z_2) \times v$ , relate the interaction parameters to the treatment-combination parameters (cf. eq. (9)), and determine the constraints on the interaction parameters due to the application of U' t = 0.

<u>Step 7</u>. Form  $\overline{\hat{a}}(X_i)$  by eliminating from  $\overline{\hat{a}}(X_i)$ ,  $i = 1, 2, ..., 2^n - 1$ , those interaction parameters equal to zero or those of highest order in the constraints determined in step 6. Similarly, form  $\overline{\overline{M}}(X_i)$  by eliminating the corresponding rows of each  $\overline{M}(X_i)$ .

Step 8. Determine the aliased or confounded effects, if any, in accordance with definitions in section 4.4.

Step 9. Compute the sums of squares and degrees of freedom for those interaction terms which have at least one parameter in  $\overline{\overline{a}}$  as indicated in section 4.3. The block, error, and total sums of squares and degrees of freedom are given in the analysis of variance table of section 4.3. If the design is orthogonal,

$$\sum_{j=1}^{s} SS\left(a\left(X_{i_{j}}\right)\right) = SS\left(t\right) = \hat{t}' Q.$$

#### 6. EXAMPLES

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In this section, we give an arbitrary example to illustrate the notation and computational procedure throughout. Then we outline solutions, using the methods of this paper, for two examples published by other investigations.<sup>16,17</sup>

Consider a two-factor experiment with factor  $A_1$  appearing at  $m_1 = 3$  levels and factor  $A_2$  at  $m_2 = 2$  levels. In accordance with section 4.1, the treatment combinations are labeled

				Treatment Combination	Tro 	Treatment Label	
$\begin{pmatrix} 1\\ 2\\ 3 \end{pmatrix}$	Ø	$\begin{pmatrix} 1\\ 2 \end{pmatrix}$	=	11 12 21 22 31 32	=	1 2 3 4 5 6	

<sup>&</sup>lt;sup>16</sup>Davies, O. L. (1967) <u>Design and Analysis of Industrial Experiments</u>, Hafner Publishing Co., New York.

<sup>&</sup>lt;sup>17</sup>Zelan, M. (1964) Applications of the Calculus for Factorial Arrangements II: Unequal Numbers in the Analysis of Variance, MRC Tech. Summary Report 411, U. S. Army Math Res. Center, Univ. of Wisc.

Suppose the original test design was, inadvertently, not executed as planned, and five of the v = 6 treatments were applied to b = 3 blocks with generalized incidence matrix,

$$\mathbf{L} = \begin{pmatrix} 2 & C & 0 \\ 1 & 0 & 0 \\ C & 1 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

What effects can now be estimated, given this poorly executed design, and with what efficiency? From this incidence matrix, one determines by inspection that  $R = \text{diag} (2 \ 1 \ 1 \ 3 \ 1 \ 0)$ ,  $K = \text{diag} (3 \ 4 \ 1)$ , the number of sets of connected blocks is  $z_1 = 3$  and the number of missing treatments is  $z_2 = 1$ . Hence by Theorem 1, the rank of the coefficient matrix C, will be  $v - z_1 - z_2 = 2$ . Computing  $C = R - LK^{-1}L'$ , one gets after reduction

$$C = \begin{pmatrix} 2/3 & M_2 & 0_2 \\ 0_2 & 3/4 & M_2 & 0_2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; M_2 = 2 I_2 - J_2 \text{ and } 0_2 \text{ are square (21)}$$
matrices of order 2.

Since C is a diagonal matrix with quasi-idempotent elements along the diagonal, the GI is computed directly as

$$\mathbf{C}^{+} = \begin{pmatrix} 3.78 \, \mathrm{M}_{2} & 0_{2} & 0_{2} \\ 0_{2} & 1.73 \, \mathrm{M}_{2} & 0_{2} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
(22)

Suppose we are given the vector of responses (cf. section 3.1)

$$Y' = (y_{111} \ y_{112} \ y_{211} \ y_{321} \ y_{421} \ y_{422} \ y_{423} \ y_{531}).$$

Then the treatment and block totals are given by

$$T_{1} = y_{111} + y_{112} \qquad B_{1} = y_{111} + y_{112} + y_{211}$$

$$T_{2} = y_{211} \qquad B_{2} = y_{321} + y_{421} + y_{422} + y_{423}$$

$$T_{3} = y_{321} \qquad B_{3} = y_{531}$$

$$T_{4} = y_{421} + y_{422} + y_{423}$$

$$T_{5} = y_{531}$$

$$T_{6} = 0$$
(23)

Then the vector of adjusted treatment totals Q is given by

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$$Q = T - LK^{-1} B = \begin{bmatrix} T_1 - 2/3 B_1 \\ T_2 - 1/3 B_2 \\ T_3 - 1/4 B_2 \\ T_4 - 3/4 B_2 \\ T_5 - B_3 \\ 0 \end{bmatrix} = \begin{bmatrix} 1/3 (y_{111} + y_{112} - 2 y_{211}) \\ 1/3 (2 y_{211} - y_{112} - y_{111}) \\ 1/4 (3 y_{321} - y_{421} - y_{422} - y_{423}) \\ 1/4 (y_{421} + y_{422} + y_{423} - 3 y_{321}) \\ 0 \\ 0 \end{bmatrix}$$
(24)

The minimum variance unbiased estimate is then given by

$$\hat{t} = C^{\dagger} Q = \begin{bmatrix} 1/4 (y_{111} + y_{112} - 2 y_{221}) \\ -1/4 (y_{111} + y_{112} - 2 y_{221}) \\ 1/6 (3 y_{321} - y_{421} - y_{422} - y_{423}) \\ -1/6 (3 y_{321} - y_{421} - y_{422} - y_{423}) \\ 0 \\ 0 \end{bmatrix}$$
(25)

The estimation of the main effect and interaction terms follows the discussion of section 4.2. The  $2^2 - 1 = 3$  effect terms are ordered lexicographically as

 $X_1 = (10)$ : main effect of factor  $A_1$ 

 $X_2 = (01)$ : main effect of factor  $A_2$ 

 $X_3 = (11)$ : two factor interaction  $A_1 A_2$ 

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In accordance with eq. (13), the minimum variance unbiased estimate for each vector  $\mathbf{X}_i$  is given by

$$\hat{a}(X_i) = \frac{1}{v} M(X_i) \hat{t} = \frac{1}{v} M(X_i) C^+ Q$$

For  $X_1 = (10)$ , one gets

$$\hat{\mathbf{a}} (\mathbf{X}_{1}) = \begin{bmatrix} \hat{\mathbf{a}}_{1} (1) \\ \hat{\mathbf{a}}_{1} (2) \\ \hat{\mathbf{a}}_{1} (3) \end{bmatrix} = \frac{1}{v} \begin{bmatrix} \mathbf{M}_{3} \times \mathbf{1}_{2}' \end{bmatrix} \hat{\mathbf{t}} = 1/6 \begin{bmatrix} 2 & 2 & -1 & -1 & -1 & -1 \\ -1 & -1 & 2 & 2 & -1 & -1 \\ -1 & -1 & 2 & 2 & -1 & -1 \\ -1 & -1 & -1 & -1 & 2 & 2 \end{bmatrix} \hat{\mathbf{t}}$$

$$= \begin{bmatrix} 2 & \hat{\mathbf{t}}_{1} + 2 & \hat{\mathbf{t}}_{2} - \hat{\mathbf{t}}_{3} - \hat{\mathbf{t}}_{4} - \hat{\mathbf{t}}_{5} - \hat{\mathbf{t}}_{6} \\ -\hat{\mathbf{t}}_{1} - \hat{\mathbf{t}}_{2} + 2 & \hat{\mathbf{t}}_{3} + 2 & \hat{\mathbf{t}}_{4} - \hat{\mathbf{t}}_{5} - \hat{\mathbf{t}}_{6} \\ -\hat{\mathbf{t}}_{1} - \hat{\mathbf{t}}_{2} - \hat{\mathbf{t}}_{3} - \hat{\mathbf{t}}_{4} + 2 & \hat{\mathbf{t}}_{5} + 2 & \hat{\mathbf{t}}_{6} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
(26)

It will be shown below that the main effect of factor  $A_1$  is totally confounded with blockshence, this null result for  $\hat{a}(X_1)$ . For  $X_2 = (01)$ , we get

$$\hat{a} (X_2) = \begin{bmatrix} \hat{a}_2 (1) \\ - \hat{a}_2 (1) \end{bmatrix} = \frac{1}{v} \begin{bmatrix} 1_3' \times M_2 \end{bmatrix} \hat{t} = 1/6 \begin{bmatrix} 1 - 1 & 1 - 1 & 1 - 1 \\ - 1 & 1 - 1 & 1 & -1 \end{bmatrix} \hat{t}$$

$$\hat{a} (X_2) = \begin{bmatrix} 1/2 (y_{111} + y_{112} - 2 y_{221}) + 1/3 (3 y_{321} - y_{421} - y_{422} - y_{423}) \\ - \hat{a}_2 (1) \end{bmatrix}$$
(27)

Finally, for  $x_3 = (11)$ , we get utilizing the constraint eq. (10)

$$\hat{a} (X_3) = \hat{a}_1 \otimes \hat{a}_2 = \begin{bmatrix} \hat{a}_{12} (11) \\ & \hat{a}_{12} (21) \\ & & \hat{a}_{12} (21) \\ & & & \hat{a}_{12} (21) \\ & & & & \\ & & - \hat{a}_{12} (21) \\ & & & & \\ & & - \hat{a}_{12} (11) - \hat{a}_{12} (21) \\ & & & & \\ & & & \\ & &$$

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It is readily verified that

$$\ddot{a}_{12}(11) = (y_{111} + y_{112} - 2 y_{221}) - 1/3 (3 y_{321} - y_{421} - y_{422} - y_{423})$$

and

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$$\hat{a}_{12} (21) = -\frac{1}{2} (y_{111} + y_{112} - 2 y_{221}) + \frac{2}{3} (3 y_{321} - y_{421} - y_{422} - y_{423})$$

Hence the  $v \sim 1 = 5$  elements of the  $\overline{a}(X)$  matrix of section 4.3 are given by

$$\overline{a}'(X) = [a_1(1) a_1(2) a_2(1) a_{12}(11) a_{12}(21)],$$
 (29)

with minimum variance unbiased estimates as given above. The corresponding  $\overline{M}(X)$  matrix is given by (cf. section 4.3)

$$\widetilde{M}(X) = \begin{bmatrix} 2 & 2 & -1 & -1 & -1 & -1 \\ -1 & -1 & 2 & 2 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 2 & -2 & -1 & 1 & -2 & 1 \\ -1 & 1 & 2 & -2 & -1 & 1 \end{bmatrix} = \begin{bmatrix} \widetilde{M}(X_1) \\ \widetilde{M}(X_2) \\ \widetilde{M}(X_3) \end{bmatrix}$$
(30)

Now, since rank  $C = (v - z_1 - z_2 = 2) < (v - 1 = 5)$ , there exist  $z_1 + z_2 - 1 = 3$  additional relationships among the elements in  $\overline{a}(X)$  that are determined from constraint equation U't = 0. In accordance with section 3.4, the constraint matrix U' is given by

[	11	00	00]
	00	11	00
U' =	00	00	10
	00	00	01

Using equation (9) and (10) we can write the vector of treatment effects in terms of the treatment combination parameters as 10-725 COTTO

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$$\begin{bmatrix} t_{1} \\ t_{2} \\ t_{3} \\ t_{4} \\ t_{5} \\ t_{6} \end{bmatrix} = \begin{bmatrix} a_{1} (1) \\ a_{1} (1) \\ a_{1} (2) \\ a_{1} (2) \\ -a_{1} (1) - a_{1} (2) \\ -a_{1} (1) - a_{1} (2) \end{bmatrix} + \begin{bmatrix} a_{2} (1) \\ -a_{2} (1) \end{bmatrix} + \begin{bmatrix} a_{12} (11) \\ -a_{12} (11) \\ -a_{12} (21) \\ -a_{12} (11) -a_{12} (21) \\ +a_{12} (11) -a_{12} (21) \end{bmatrix}$$
(32)

We get from U't = 0 after reduction

$$a_1(1) = a_1(2) = 0$$
  
 $a_{12}(21) = a_2(1) - a_{12}(11)$ 
  
(33)

Hence, the v -  $z_1 - z_2 = 2$  estimable parameters that make up the  $\overline{a}$  (X) matrix are

$$\overline{\hat{a}}'(X) = [\hat{a}_{2}(1) \hat{a}_{12}(11)].$$
 (34)

The minimum variance estimates for the elements of  $\overline{\tilde{a}}(X)$  are given in eq. (27) and (28). Retaining the rows of  $\overline{M}(X)$  associated with the two elements of  $\overline{\tilde{a}}(X)$  there results

$$\overline{\overline{M}}(X) = \begin{bmatrix} 1 & -1 & 1 & -1 & 1 & -1 \\ & & & & \\ 2 & -2 & -1 & 1 & -1 & 1 \end{bmatrix} = \begin{bmatrix} \overline{\overline{M}}(X_2) \\ \\ \\ \\ \overline{\overline{M}}(X_3) \end{bmatrix}$$
(35)

The aliasing and confounding is determined from eq. (33). Using definition 3, section 4.4, and the first equation of (33), the main effect of factor  $A_1$  is found to be completely confounded with blocks. The second relation in eq. (33) reveals through definition 2 of section 4.4 that the two factor interaction  $A_1 A_2$  is aliased with the main effect of factor  $A_2$  as well as with itself.

The variance-covariance matrix for the independent estimable parameters is given by eq. (20).

$$\overline{\overline{V}} = \frac{\sigma^2}{v^2} \overline{\overline{M}} (X) C^* \overline{\overline{M}}' (X) = \begin{bmatrix} Var \overline{\overline{a}} (X_2) Cov [\overline{\overline{a}} (X_2), \overline{\overline{a}} (X_3)] \\ Cov [\overline{\overline{a}} (X_2), \overline{\overline{a}} (X_3)] Var \overline{\overline{a}} (X_3) \end{bmatrix}$$

$$= \frac{\sigma^2}{36} \begin{bmatrix} \frac{17}{6} & \frac{5}{3} \\ \frac{5}{3} & \frac{22}{3} \end{bmatrix}$$
(36)

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Using eq. (20) and (36)

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$$\overline{\overline{\Sigma}} (X_2) = \operatorname{Var} \overline{\overline{a}} (X_2) = \frac{17}{216}$$

$$\overline{\overline{\Sigma}} (X_3) = \operatorname{Var} \overline{\overline{a}} (X_3) = \frac{22}{108}$$
(37)

Using eq. (34), (20) and (37), the effect sums of squares are now computed as

$$SS(a(X_{2})) = \overline{\tilde{a}}'(X_{2}) [\overline{\Sigma}(X_{2})]^{-1} \overline{\tilde{a}}(X_{2}) = \frac{216}{17} \hat{a}_{2}^{2} (1)$$

$$SS(a(X_{3})) = \overline{\tilde{a}}'(X_{3}) [\overline{\Sigma}(X_{3})]^{-1} \hat{a}(X_{3}) = \frac{108}{22} \hat{a}_{12}^{2} (11)$$
(38)

where  $\hat{a}_2(1)$  and  $\hat{a}_{12}(11)$  are evaluated in eq. (27) and (28), respectively.

We note in eq. (36) that the covariance between the effect terms  $A_1$  and  $A_1A_2$  is not zero. Therefore, the design is not orthogonal, and the sums of squares in eq. (38) cannot be expected to sum to the sums of squares for treatments, t'Q. Finally, from section 4.3, the analysis of variance table is evaluated as

Source	Sums of Squares	d.f.	
$X_2$ : main effect of $A_2$	$SS(a(X_2)) = \frac{216}{17} [a_2(1)]^2$	$\operatorname{rank}\overline{\overline{\Sigma}}(X_2) = 1$	
$X_3$ : interaction $A_1 A_2$	$SS(a(X_3)) = \frac{108}{22} [a_{12}(11)]^2$	rank $\overline{\overline{\Sigma}}$ (X <sub>3</sub> ) = 1	
Blocks	B'K <sup>-1</sup> B	b - 1 = 2	
Error	$\mathbf{Y'}\mathbf{Y} - \mathbf{\hat{t}'}\mathbf{Q} - \mathbf{B'}\mathbf{K}^{-1}\mathbf{B}$	w-rank $C - b = 3$	
Total	Y'Y - G <sup>2</sup> /w	7	

The following two examples have been extracted from Davies<sup>16</sup> and Zelen.<sup>17</sup> The solutions are given in abbreviated form somewhat in the form of the output of the computer program available for this analysis. Hopefully, the detailed solution for the prior example will be sufficient to make clear the brief annotations to these examples.

They are included here to facilitate the relating and contrasting of the solutions using the methods of this paper to those using other possible techniques.

<sup>16</sup>Dovies, O. L. (1967) Design and Analysis of Industrial Experiments, Hafner Publishing Co., New York, 466.
 <sup>17</sup>Zelen, M. (1964) Applications of the Calculus for Factorial Arrangements II: Unequal Numbers in the

Analysis of Variance, MRC Tech. Summary Repirt 411, U.S. Army Math. Res. Center, Univ. of Wisc.

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#### Example 2: One-half Fraction of 2<sup>5</sup> Design, Davies<sup>16</sup>

Number of Factors $(n) = 5$				
Factor (A,)/I	ævels (m,)			
Α,	2			
A <sub>2</sub>	2			
A,	2			
A 🕺	2			
A	2			

Number of treatments (v) = 32Number of Blocks (b) = 4

Treatment <sup>†</sup> Label	Treatment Combination $(i_1, i_2, i_3, i_4, i_5)$	Generalized Incidence Matrix (L*) <sup>1</sup>	Vector of Observations (Y)
2	11112	0001	$y_{2,4,1} = 775$
3	11121	1000	y, = 819
5	11211	0010	$y_{5,3,1} = 593$
8	11222	0100	$y_{8,2,1} = 878$
9	12111	0100	$y_{9} = 756$
12	12122	0010	y <sub>12</sub> , = 745
14	12212	1000	y, , = 785
15	12221	0 0 0 1	$y_{15,4,1} = 851$
17	21111	1000	y <sub>17</sub> , 1 = 625
20	21122	0 0 0 1	$y_{20}$ , = 735
22	21212	0100	$y_{11} = 625$
23	21221	0010	y <sub>22</sub> = 656
26	22112	0010	$y_{26-3-1} = 666$
27	22121	0100	y <sub>27,2,1</sub> = 841
29	22211	0 0 0 1	$y_{29,4,1} = 628$
32	22222	1000	$y_{32,1,1} = 732$

 $R^* = I_{16}^{\dagger}$ ; K = 4 $J_4$ ;  $z_1 = 4$ ;  $z_2 = 16$ 

<sup>†</sup> Troatments labeled, 1,4,6,7,10,11,13,16,18,19,21,24,25,28,30, and 31 are missing from the experiment.

 $L^* = L$  with rows corresponding to missing treatments deleted.

 $R^* = R$  with rows and columns corresponding to missing treatments deleted.

$$C^* = R^* - L^* K^{-1} L'$$

$C^{\bullet} = \frac{1}{4}$	3 I <sub>4</sub>	$(I_2 - J_2) \times (I_2 - J_2)$	$I_2 < (I_2 - J_2)$	$(I_2 - J_2) \times I_2$
	$-(\mathbf{I}_2 - \mathbf{J}_2) \times (\mathbf{I}_2 - \mathbf{J}_2)$	3 I <sub>4</sub>	$(I_2 - J_2) \times I_2$	$I_2 < (I_2 - J_2)$
	$\mathbf{I_2} \times (\mathbf{I_2} - \mathbf{J_2})$	$(I_2 - J_2) \times I_2$	3 I <sub>4</sub>	$-(\mathbf{I}_2 - \mathbf{J}_2) \times (\mathbf{J}_2 - \mathbf{J}_2)$
	$(I_2 - J_2) \times I_2$	$\mathbf{I_2}\times(\mathbf{I_2}-\mathbf{J_2})$	$-(I_2 - J_2) \times (I_2 - J_2)$	3 I <sub>4</sub>

 $C^*$  is idempotent;  $C^{*+} = C^*$ 

 $Q^{*'} = \{T^{*} - L^{*}K^{-1}B\}^{'} = \frac{1}{4} [111,315,-238,412,-76,320,179,415,-461,-49,-600,-36,4,264,-477,-33]$  $\hat{t}^{*} = C^{*} Q^{*} = Q^{*}$ 

Rank  $C = v - z_1 - z_2 = 12 = degrees of freedom for treatments$ 

 $SS(t) = \hat{t}^* Q^* = 96951.5 \cdot \hat{t} Q = \text{treatment sums of squares}$ 

- Note: 1. The starred vectors (matrices) are the unstarred counterparts with rows (rows and columns) associated with missing treatments deleted. The deleted rows (rows and columns) contain zero elements only.
  - 2. Subscripts on partitions of C\* denote the dimensions of the indicated square matrices.

<sup>16</sup>Davies, O. L. (1967 <u>Design and Analysis of Industrial Experiments</u>, Hafner Publishing Co., New York, 465.

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## $\hat{a}(X) = M^{*}(X)\hat{t}^{*}/v = M(X)\hat{t}/v^{\dagger \dagger}$

Interaction Effect Vectors

Levels of Factors

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Star Strategy

	â	t L	a2	â,	_	â <sub>4</sub>	âs	
1 2	$\frac{347}{16} \bigg[ -$	$\begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 14 \\ 1 \end{bmatrix}$	$\frac{9}{6}\begin{bmatrix}-1\\1\end{bmatrix}$	$\frac{107}{16} \begin{bmatrix} 1\\ -1 \end{bmatrix}$	$\frac{402}{10}$	$\begin{bmatrix} 2 \\ -1 \\ 1 \end{bmatrix}$	$\frac{86}{16} \begin{bmatrix} -1\\1 \end{bmatrix}$	∫a, (1)
	â <sub>12</sub>	â	â <sub>14</sub>	â <sub>15</sub>	â. <sub>24</sub>	â <sub>34</sub>	â <sub>45</sub>	$\begin{vmatrix} a_{2}(1) \\ a_{3}(1) \end{vmatrix}$
11 12 21 22	$\frac{77}{16} \begin{bmatrix} 1\\ -1\\ -1\\ 1 \end{bmatrix}$	$\frac{119}{16} \begin{bmatrix} -1\\ 1\\ 1\\ -1\\ -1 \end{bmatrix}$	$\frac{18}{16} \begin{bmatrix} 1\\ -1\\ -1\\ 1\\ 1 \end{bmatrix}$	$\frac{78}{16} \begin{bmatrix} -1\\1\\1\\-1 \end{bmatrix}$	$\frac{68}{16} \begin{bmatrix} -1 \\ 1 \\ 1 \\ -1 \end{bmatrix}$	$\frac{84}{16} \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix}$	$\frac{163}{16} \begin{bmatrix} -1\\ 1\\ 1\\ -1 \end{bmatrix}$	$ \begin{array}{c}     a_{4}(1) \\     a_{5}(1) \\     a_{12}(11) \\     a_{13}(12) \\     a_{14}(11) \end{array} $
	â <sub>123</sub>	ā <sub>125</sub>	â <sub>135</sub>	a234	â <sub>235</sub>	â <sub>245</sub>	â <sub>345</sub>	$a_{15}(11)$ $a_{1,1}(11)$
111 112 121 122 211 212 221 222	$ \begin{array}{c} 1 \\ -1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ 1 \\ -1 \end{array} $	$ \begin{array}{c}                                     $	$\begin{array}{c} 1\\ -1\\ -1\\ 1\\ 1\\ -1\\ 1\\ 1\\ -1\\ \end{array}$	$ \begin{array}{c} 1 \\ -1 \\ -1 \\ 1 \\ 1 \\ -1 \\ 1 \\ 1 \\ -1 \end{array} $	$\frac{18}{16} \begin{bmatrix} -1\\ 1\\ 1\\ -1\\ 1\\ -1\\ 1\\ -1\\ 1 \end{bmatrix}$	$\underbrace{\frac{119}{16}}_{16}\begin{bmatrix}1\\-1\\-1\\1\\-1\\1\\1\\1\\-1\end{bmatrix}}$	$\frac{77}{16}\begin{bmatrix} -1\\1\\1\\-1\\1\\-1\\1\\-1\\-1\\1\end{bmatrix}$	$\mathbf{a} = \begin{bmatrix} \mathbf{a}_{24}^2 (11) \\ \mathbf{a}_{25}^2 (11) \\ \mathbf{a}_{34}^2 (11) \\ \mathbf{a}_{35}^2 (11) \\ \mathbf{a}_{45}^2 (11) \\ \mathbf{a}_{123}^2 (111) \\ \mathbf{a}_{124}^2 (111) \\ \mathbf{a}_{125}^2 (111) \\ \mathbf{a}_{134}^2 (111) \end{bmatrix}$
	Â <sub>1234</sub>	â <sub>1235</sub>	ł	1245	â <sub>1345</sub>	â	2345	$a_{135}$ (111) $a_{135}$ (111)
1111 1112 1121 1122 1211 1212 1221 1222 2111 2122 2121 2122 2211 2212 2221	$ \begin{array}{c} 1\\ -1\\ -1\\ 1\\ -1\\ 1\\ 1\\ -1\\ 1\\ 1\\ -1\\ 1\\ -1\\ -$	$\begin{bmatrix} 1\\ -1\\ -1\\ 1\\ -1\\ 1\\ -1\\ 1\\ -1\\ 1\\ 1\\ -1\\ 1\\ -1\\ 1\\ -1\\ -$	<u>107</u> 18	-1 1 1 -1 -1 -1 -1 -1 -1 -1 -1	$ \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ 1 \\ -1 \\ 1 \\ -1 \\ -$	<u>347</u> 16	-1 1 1 -1 -1 -1 -1 -1 -1 -1 -1	$\begin{array}{c} a_{234}^{123} (111) \\ a_{235}^{234} (111) \\ a_{235}^{235} (111) \\ a_{345}^{245} (111) \\ a_{1234}^{1234} (1111) \\ a_{1235}^{1235} (1111) \\ a_{1245}^{12345} (1111) \\ a_{2345}^{2345} (1111) \\ a_{12345}^{12345} (1111) \end{array}$

 $a_{23} = a_{25} = a_{35} = a_{124} = a_{134} = a_{145} = a_{12345}$  are zero vectors † To be read  $\hat{a}_1' = [\hat{a}_1(1)\hat{a}_1(2)] = \frac{347}{16} \{1, -1\} = \{21, 7, -21, 7\}$ 

 $^{\dagger\dagger}$  M\*(X) is formed by deleting columns (only) of M(X) associated with missing treatments.

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Constraint Matrix U':

Dependency Relationships found from:

 $\mathbf{U}'\mathbf{t} = \mathbf{U}' \sum_{n=1}^{n} \sum_{\lambda = 1}^{n} \mathbf{a}_{1}(\alpha_{1}) * \dots * \mathbf{a}_{n}(\alpha_{n}) = 0$ Formed so that U't = 0 yields:  $t_3 + t_{14} + t_{17} + t_{32} = 0$  $t_8 + t_9 + t_{22} + t_{27} = 0$  $t_5 + t_{12} + t_{23} + t_{26} = 0$ a<sub>23</sub> (11) = 0  $t_2 + t_{15} + t_{20} + t_{29} = 0$  $a_{25}(11) = 0$  $t_1 = t_4 = t_6 = t_7 = t_{10} = t_{11} = t_{13} = t_{16} = 0$ a35 (11) = 0  $\mathbf{t}_{18} = \mathbf{t}_{19} = \mathbf{t}_{21} = \mathbf{t}_{24} = \mathbf{t}_{25} = \mathbf{t}_{28} = \mathbf{t}_{30} = \mathbf{t}_{31} = \mathbf{0}$  $a_{123}$  (111) =  $-a_{45}$  (11) Factors Confounded a,24 (111) = 0 Factors/Aliases With Blocks a<sub>125</sub> (111) = -a<sub>34</sub> (11) a, (1) A, A<sub>2</sub>A<sub>3</sub>A<sub>4</sub>A<sub>5</sub>  $A_2A_3$  $a_{134}(111) = 0$  $A_2 A_1 A_3 A_4 A_5$ a2(1) A,A.  $a_{135}(111) = -a_{24}(11)$ a<sub>3</sub> (1) **A**<sub>3</sub> A<sub>1</sub>A<sub>2</sub>A<sub>4</sub>A<sub>5</sub> A<sub>3</sub>A<sub>5</sub> A.  $A_1A_2A_3A_5$ a<sub>4</sub>(1) A, A, A a (111) = 0  $A_1A_2A_3A_4$ a<sub>5</sub> (1) A, A, A, A<sub>5</sub> a234 (111) = -a15 (11)  $a_{12}(11)$  A, A, A, A, A, A, A, A1A4A5  $\bar{\bar{a}} = |a_{13}(11)| A_1 A_3$ A<sub>2</sub>A<sub>4</sub>A<sub>5</sub>  $A_1A_2A_3A_4A_5$  $a_{235}(111) = -a_{14}(11)$  $a_{14}(11) = A_1A_4 = A_2A_3A_5$  $a_{245}(111) = -a_{13}(11)$  $a_{15}(11) = A_1A_5 = A_2A_3A_4$  $q_{345}(111) = -a_{12}(11)$ a24 (11)  $A_2A_4 - A_1A_3A_5$ a<sub>34</sub> (11)  $A_3A_4 = A_1A_2A_5$  $a_{1234}(1111) = -a_5(1)$ a45 (11) A<sub>4</sub>A<sub>5</sub> A<sub>1</sub>A<sub>2</sub>A<sub>3</sub>  $a_{1235}(1111) = -a_4(1)$ .  $a_{1245}(1111) = -a_3(1)$  $a_{1345}(1111) = -a_2(1)$  $a_{2345}(1111) = -a_1(1)$ 

a<sub>12345</sub> (11111) = 0

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Variance-Covariance Matrix

$$\overline{V}/\sigma^2 = \overline{\Sigma}^{\dagger} = \frac{1}{64} I_{12} = \frac{1}{\sigma^2} \begin{pmatrix} \text{Var } \hat{a}_1 (1) \\ \text{Var } \hat{a}_2 (1) & 0 \\ 0 & \text{Var } \hat{a}_{34} (11) \\ \text{Var } \hat{a}_{45} (11) \end{pmatrix}$$

Design is orthogonal.

$$SS\left[a\left(X_{i_{j}}\right)\right] = \overline{\tilde{a}}^{\prime}\left(X_{i_{j}}\right) \overline{\Sigma}\left(X_{i_{j}}\right)^{-1} \overline{\tilde{a}}\left(X_{i_{j}}\right) = \overline{\tilde{a}}^{2}\left(X_{i_{j}}\right) \cdot 64$$

$$Degrees of freedom for \overline{\tilde{a}}\left(X_{i_{j}}\right) = Rank \overline{\Sigma}\left(X_{i_{j}}\right) = 1$$

## Analysis of Variance Table

Source of Variation	Sums of Squares	Degrees of Freedom
A <sub>1</sub>	30102.25	1
A <sub>2</sub>	5550.25	1
A <sub>3</sub>	2862.25	1
A <sub>4</sub>	40401.00	1
Ag	1849.00	1
A <sub>1</sub> A <sub>2</sub>	1482.25	1
A <sub>1</sub> A <sub>3</sub>	3540.25	1
A <sub>1</sub> A <sub>4</sub>	81.00	1
A <sub>1</sub> A <sub>5</sub>	1521.00	1
A <sub>2</sub> A <sub>4</sub>	1156.00	1
A <sub>3</sub> A <sub>4</sub>	1764.00	. 1
A <sub>4</sub> A <sub>5</sub>	6642.25	1
Blocks	26554.25	3
Total	123505.75	15

Rows and columns of  $\overline{\overline{V}}$  associated with elements of  $\overline{a}$ .

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## EXAMPLE 3: A 3 $\times$ 2 $\times$ 2 FACTORIAL WITH UNEQUAL NUMBER, ZELEN<sup>17</sup>

Number of Factors (n) = 3

Number of Treatments (v) = 12

Number of Blocks (b) = 1

Factor  $(A_i)$ /Levels  $(m_i)$ 

A<sub>1</sub> 3 A<sub>2</sub> 2 A<sub>3</sub> 2

Treatment Label	Treatment Combination $(i_1, i_2, i_3)$	Generalized Incidence Matrix (L)	Vector of Observations (Y)
1	111	1	y,, = 5
2	112	1	$y_{2,1,1} = 5$
3	121	2	$y_{3,1,1} = 10$
4	122	2	$y_{3.1.2} = 12$ $y_{4.1.1} = 13$ $y_{4.1.2} = 17$
5	211	1	$y_{5,1,1} = 9$
6	212	1	$y_{6,1,1} = 9$
7	221	1	$y_{7,1,1} = 7$
8	222	2	$y_{8,1} = 14$
9	311	3	$y_{8,1,2} = 16$ $y_{0,1,1} = 9$ $y_{9,1,2} = 13$ $y_{0,1,2} = 8$
10	312	1	y = 10
11	321	1	y, , = 12
12	322	1	$y_{12,1,1} = 12$

$$R = diag (1 \ 1 \ 2 \ 2 \ 1 \ 1 \ 1 \ 2 \ 3 \ 1 \ 1 \ 1)$$

K = 17

 $z_1 = 1; z_2 = 0$ 

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<sup>&</sup>lt;sup>17</sup>Zelen, M. (1964) Applications of the Calculus for Factorial Arrangements II: Unequal Numbers in the Analysis of Variance, MRC Tech. Summary Report 411, U.S. Army Math Res. Center, Univ. of Wisc.

$$C = R - LK^{-1}L' = \frac{1}{17} \begin{bmatrix} 17 I_2 - J_2 & -2 J_2 & -J_{2 \times 3} & (-2I_2: -3I_2) & -J_{2 \times 3} \\ -2 J_2 & 34 I_2 - 4 J_2 & -2 J_{2 \times 3} & (-4I_2: -6I_2) & -2 J_{2 \times 3} \\ -J_{3 \times 2} & -2 J_{3 \times 2} & 17 I_3 - J_3 & (-2I_3: -3I_3) & -J_3 \\ \begin{pmatrix} -2I'_2 \\ \cdot \\ \cdot \\ -3I'_2 \end{pmatrix} & \begin{pmatrix} -4I'_2 \\ \cdot \\ -6I'_2 \end{pmatrix} & \begin{pmatrix} -2I'_3 \\ \cdot \\ -3I'_3 \end{pmatrix} & \begin{pmatrix} 30 & -6 \\ \\ -6 & 42 \end{pmatrix} \begin{pmatrix} -2I'_3 \\ \cdot \\ -3I'_3 \end{pmatrix} \\ \begin{pmatrix} -2I'_3 \\ \cdot \\ -3I'_3 \end{pmatrix} & \begin{pmatrix} -I_3 \\ -I_3 \\ -I_3 \\ -I_3 \\ -I_3 \end{pmatrix} \end{bmatrix}$$

C is not idempotent.

$$C^{*} = \frac{1}{864} \begin{bmatrix} 864 I_{2} - 85 J_{2} & -49 J_{2} & 85 J_{2 \times 3} & (-491_{2}: -371_{2}) & -85 J_{2 \times 3} \\ -49 J_{2} & 432 I_{2} - 13 J_{2} & -49 J_{2 \times 3} & (-131_{2}: -1_{2}) & -49 J_{2 \times 3} \\ -85 J_{3 \times 2} & -49 J_{3 \times 2} & 864 I_{3} - 85 J_{3} & (-491_{3}: -371_{3}) & -85 J_{3} \\ \begin{pmatrix} -491_{2}' \\ \cdot \\ -371_{2}' \end{pmatrix} & \begin{pmatrix} -131_{2}' \\ \cdot \\ -1_{2}' \end{pmatrix} & \begin{pmatrix} -491_{3}' \\ \cdot \\ -371_{3}' \end{pmatrix} & \begin{pmatrix} 419 & -1 \\ \\ -1 & 299 \end{pmatrix} & \begin{pmatrix} -491_{3}' \\ \cdot \\ -371_{3}' \end{pmatrix} \\ -85 J_{3 \times 2} & -49 J_{3 \times 2} & -85 J_{3} & (-491_{3}: -371_{3}) & 864 I_{3} - 85 J_{3} \end{bmatrix}$$

$$Q' = (T - LK^{-1}B)' = (T - \frac{G}{17}L)'$$

 $=\frac{1}{17} (-96 \quad -96 \quad 12 \quad 148 \quad -28 \quad -28 \quad -62 \quad 148 \quad -33 \quad -11 \quad 23 \quad 23)$ 

 $\hat{\mathbf{t}}' = (\mathbf{C}^+ \mathbf{Q})' = (-5 \ -5 \ 1 \ 5 \ -1 \ -1 \ -3 \ 5 \ 0 \ 0 \ 2 \ 2)$ 

Rank C = v -  $z_1 - z_2 = 11$  degrees of freedom for treatments SS(t) =  $\hat{t}' Q = 163.882$ 

Levels of Factors	Interaction Effect	$\hat{a}(X) = M(X)\hat{t}/v$	
1 2 3	$\begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} -2 \\ 2 \end{bmatrix}$	$a_3$ $\begin{bmatrix} -1\\1 \end{bmatrix}$	$\begin{bmatrix} a_1(1) \\ a_2(2) \end{bmatrix}$
11 12 21 22 31 32	$ \begin{array}{c} \mathbf{a_{12}} & \mathbf{a_{13}} \\ \begin{bmatrix} -2 \\ 2 \\ 1 \\ -1 \\ 1 \\ -1 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ -1 \\ 1 \\ 1 \\ 1 \\ -1 \end{bmatrix} $	a <sub>23</sub> $ \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix} $	$\vec{a} = \begin{bmatrix} a_{1}(2)' \\ a_{2}(1) \\ a_{3}(1) \\ a_{12}(21) \\ a_{13}(21) \\ a_{13}(21) \\ a_{13}(21) \\ a_{23}(11) \\ a_{123}(211) \end{bmatrix}$
111 112 121 122 211 212 221 222 311 312 321 322	$ \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ -1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \end{bmatrix} $		$\overline{\overline{\mathbf{a}}} = \overline{\mathbf{a}}$

$$\overline{\overline{V}}/\sigma^2 = \overline{\overline{\Sigma}}^{\dagger} = \frac{1}{864} \begin{bmatrix} \overline{113} & -58 & 13 & 1 & 23 & -22 & -1 & -10 & 7 & -7 & 2 \\ 122 & 4 & 10 & -22 & 14 & -10 & 8 & -2 & 2 & -16 \\ 59 & -7 & -5 & 4 & 7 & -2 & -1 & 1 & 10 \\ 59 & 7 & -2 & -5 & 4 & 5 & 13 & 4 \\ 113 & -58 & -7 & 2 & 1 & -1 & -10 \\ 122 & 2 & -16 & 10 & -10 & 8 \\ 113 & -58 & 13 & 23 & -22 \\ 122 & 4 & -22 & 14 \\ 59 & -5 & 4 \\ 113 & -58 \\ 122 \end{bmatrix}$$

Design is not orthogonal.

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$$SS\left[a\left(X_{i_{j}}\right)\right] = \overline{\hat{a}}'\left(X_{i_{j}}\right) \overline{\Sigma}\left(X_{i_{j}}\right)^{-1} \overline{\hat{a}}\left(X_{i_{j}}\right)$$

$$Degrees of freedom for \overline{\hat{a}}\left(X_{i_{j}}\right) = Rank \overline{\Sigma}\left(X_{i_{j}}\right)$$

$$Analysis of Variance Table$$

Source of Variation	Sums of Squares	Degrees of Freedom	
A <sub>1</sub>	10.114	2	
A <sub>2</sub>	58,576	1	
A <sub>3</sub>	14.644	1	
A <sub>1</sub> A <sub>2</sub>	30.591	2	
A <sub>1</sub> A <sub>3</sub>	. 9.368	2	
A <sub>2</sub> A <sub>3</sub>	14.644	1	
A <sub>1</sub> A <sub>2</sub> A <sub>3</sub>	9,368	2	
Error	26.000	5	
Total	189.882	16	

<sup>†</sup>Rows and columns of  $\overline{\overline{V}}$  associated with elements of  $\overline{\overline{a}}$ .

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