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RESULTS ON NON-ORTHOGONAL INCOMPLETE FACTORIAL DESIGNS

STEVE R. WEBB
ROCKETDYNE, A DIVISION OF NORTH AMERICAN AVIATION, INC.
CANOGA PARK, CALIFORNIA

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FOREWORD

The three papers which this interim report comprises were written under Contract AF 33(615)-2818 entitled "Research in Experimental Design and Estimation Theory". The work, which is documented under Project 7071, Research in Applied Mathematics, was sponsored by Aerospace Research Laboratories, Office of Aerospace Research, United States Air Force, and was monitored by Dr. H. L. Harter of these Laboratories.

The first paper, entitled "Construction and Comparison of Non-Orthogonal Incomplete Factorial Designs" was prepared for presentation at the Eleventh Conference on the Design of Experiments in Army Research, Development, and Testing, held in October of 1965 at Hoboken, and appears in the proceedings of that conference. The second paper "Non-Orthogonal Designs of Even Resolution," was presented at the annual meeting of the American Statistical Association at Los Angeles in August 1966. The third paper, "Saturated Sequential Factorial Designs," represents simplification and generalization of work contained in the paper "Designs for Studying One Factor at a Time" which was presented at the Berkeley meeting of the Institute of Mathematical Statistics in July of 1965.

ABSTRACT

This report consists of three distinct but related papers. Experience in industrial consulting indicates that the requirements of a real test plan often differ from textbook examples in the number of levels for the factors, the interactions which must be estimated, and the total number of runs which can be allocated to the experiment. The first paper is concerned with methods for constructing designs to meet such requirements and with criteria for selecting a design from a number of alternatives. Various construction techniques are illustrated by examples. Two specific numerical criteria are developed, and a convenient computer routine for evaluating them is described. Examples of designs are given which were constructed for actual experiments.

In general, designs of even resolution have the property that not all the parameters are estimable, but those of primary interest are estimable with none of the remaining parameters as aliases. The most important are designs of resolution 4, which are such that the main effects are estimable with no two-factor interactions as aliases. In the second paper it is shown that the smallest resolution 4 designs for n factors at two levels must contain at least $2n$ runs, and that "foldover" designs are available with $2n$ runs. It is conjectured that the only minimal resolution 4 designs are foldover designs. The case of resolution 6 designs is also discussed.

Statistical designs which vary one factor at a time are inefficient and suffer from lack of opportunity for randomization. In spite of these deficiencies, they may be useful designs early in experiments because they yield information after each run. The third paper gives variance bounds for estimates of main effects using one-at-a-time designs, and characterizes those designs which achieve the lower bounds. Situations in which runs are conducted a block at a time (rather than singly) are discussed. Finally, it is shown that inclusion of interaction terms in the model improves the main-effect estimates of factors involved in the interactions.

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CONSTRUCTION AND COMPARISON OF NON-ORTHOGONAL INCOMPLETE FACTORIAL DESIGNS

INTRODUCTION AND SUMMARY

Very often in industrial research an experimental program must be planned for which existing fractional factorial designs are inadequate. The most common reasons for this inadequacy are

1) the available designs contain too many runs,
2) the factors to be evaluated in the experiment do not all appear at the same numbers of levels, and
3) the particular set of interactions which cannot be ignored in the analysis of the experimental results does not appear in any of the published designs.

In such cases the consulting statistician may have a tendency to try to alter the thinking of the experimenter so that one of the standard published designs can be used. This is, of course, undesirable from the experimenter's point of view and increases the probability that the design will not be carried out as originally planned. As an alternative, the statistician is faced with the problem of developing an ad hoc test plan which satisfies the actual objectives and constraints of the real situation. Using his intuition supplemented by a meager amount of theory he must come up with a design with satisfactory statistical properties.

CRITERIA FOR COMPARING DESIGNS

The response from an experiment will be denoted by the N-component vector Y, and its expected value by $EY = X\beta$, where β is a p-component vector of parameters. Generally speaking, a good design will have low parameter-estimate variances, which are proportional to the diagonal elements of $(X'X)^{-1}$. For a given experimental situation, that is, specification of the number of factors, numbers of levels for each factor, and the interactions to be estimated, a particular finite set of designs is available. In case one of these designs leads to the minimization of the variance of each estimate, then there is no selection problem. This does not often happen, however, except for fractional factorials with all factors at two levels.

In rare cases the relative importance of the parameters to be estimated may be known quantitatively well enough in advance so that a realistic criterion can be established based on the variances. This would usually take the form of a weighted average of the variances. Most often, however, the relative importance of estimating the parameters with low variances will depend on their as yet unknown values.

A criterion for selecting the design often proposed is the generalized variance, defined as the determinant of $(X'X)^{-1}$. A confidence set for the parameters is the set for which $(\beta-\hat{\beta})'(X'X)(\beta-\hat{\beta}) < K$. The volume of this ellipsiod is

$$V = \frac{2\pi^{\frac{1}{2}p} K^{\frac{1}{2}p}}{p\Gamma(\frac{1}{2}p)\sqrt{\det(X'X)}} ,$$

which is seen to be related to the design only through the determinant of the cross-product matrix. It is convenient to consider the determinant in the form of an index, called the estimation index, defined by

$$I_E = \det(X'X)/(N^p \Pi_{i=1}^p w_i) .$$

The weights w_i are defined as follows. Let Z be the coefficient matrix associated with the full factorial; that is, if Y^* were a vector of responses for a full factorial then $EY^* = Z\beta$. (The standard parameterization is such that $Z'Z$ is a diagonal matrix.) Let d_i represent the i-th diagonal entry of $Z'Z$ and let M represent the total number of runs in the full factorial. Then $w_i = d_i/M$.

Often the purpose of an experiment is to obtain overall information about the response. In these cases the appropriate criterion is based on the average variance of a fitted response, where the average is taken over all M points of the full factorial. The average variance is proportional to $\Sigma w_i V_i$, where the V_i are the diagonal elements of $(X'X)^{-1}$. A convenient representation is through the "fitting index"

$$I_F = p/(N\Sigma_{i=1}^{p} w_i V_i) \quad .$$

More generally, an index could be based on the integrated variance of a fitted response. Such an index would in general involve off-diagonal elements of $(X'X)^{-1}$, and would be difficult to define in a way which is general enough for both quantitative and qualitative factors. Experience has showed I_F to be a very useful index.

Consider the class of models which is "complete" in the sense that if any interactions between a pair of factors appear in the model, then all interactions between them appear. It has been proved [1] that for models which are complete in this sense, the maximum value of both I_E and I_F is unity. In [2] it is shown that the maximum is achieved if certain combinations of levels appear with equal frequency. An equivalent criterion is that the cross-product matrix $X'X$ is proportional to the cross-product matrix $Z'Z$ for the full factorial. All regular fractional factorials have this property. If interaction parameters do not appear in complete sets, either or both indices may be greater than unity.

Thus far nothing has been said about the parameterization used to describe the response, that is, how β is defined in terms of the expected responses at the various treatment combinations, or equivalently, how the elements of the X matrix are defined. Since the parameterization is to a large extent arbitrary, a particularly appealing property of the two indices is that they are invariant under nonsingular reparameterizations. That is, suppose $EY = X\beta = XA\alpha$, and similarly $EY^* = Z\beta = ZA\alpha$, where A is nonsingular. It can be demonstrated that I_F and I_E are identical whether calculated under the parameterization β or α. Thus, the parameterization is immaterial as far as these criteria are concerned.

Without the use of electronic computers, the computation of the indices would be extremely tedious. A computer code has been written for routine and convenient comparison of alternative incomplete factorial designs. A detailed description of this code and its use is available [3]. Any number of designs may be evaluated simultaneously by reading into the computer the treatment combinations in each. The evaluation will be made for up to five models (specification of interaction terms to be included in the model). A number of options is available to the user, including changing the parameterization used for two-, three-, or four-level factors, or changing the weights used in computing the indices. A Fortran listing is included in reference [3].

METHODS OF CONSTRUCTION

1. Exhaustive Enumeration

For a few simple experimental situations it is feasible to enumerate all possible designs. The optimum design can then easily be chosen. As an example, consider as an experimental situation a 2^3 in 5 runs with no interactions. There are exactly eleven nonsingular designs, which together with their properties are given in Table I. Clearly, the best designs are the eighth and ninth, for which each variance is minimized.

2. One Parameter at a Time

It is always possible to construct a saturated design (although they are very inefficient) by allocating one run to the estimation of each parameter. For example, a $3^2 \times 2^2$ with the linear-by-linear interaction between the two three-level factors is as follows

0 0 0 0	mean
1 0 0 0	effects of first factor
2 0 0 0	
0 1 0 0	effects of second factor
0 2 0 0	
2 2 0 0	interaction
0 0 1 0	effect of third factor
0 0 0 1	effect of fourth factor ,

where we have indicated the parameter estimated from each run. The fitting and estimation indices are .24 and .025, respectively.

TABLE I

EXHAUSTIVE ENUMERATION OF 2 CUBED IN 5 RUNS

PARAMETER	1ST DESIGN	2ND DESIGN	3RD DESIGN	4TH DESIGN	5TH DESIGN	6TH DESIGN
MEAN	0.875000	0.500000	0.875000	0.375000	0.500000	0.375000
A1	0.375000	0.375000	0.500000	0.875000	0.875000	0.500000
B1	0.375000	0.500000	0.500000	0.375000	0.500000	0.500000
C1	0.375000	0.375000	0.375000	0.375000	0.375000	0.375000
ESTIMATION INDEX	0.204800	0.204800	0.204800	0.204800	0.204800	0.204800
FITTING INDEX	0.400000	0.457143	0.355556	0.400000	0.355556	0.457143
N	5	5	5	5	5	5
DESIGNS	1) 0 0 0 2) 0 0 0 3) 0 0 1 4) 0 1 0 5) 1 0 0	1) 0 0 0 2) 0 0 0 3) 0 0 1 4) 0 1 1 5) 1 0 0	1) 0 0 0 2) 0 0 1 3) 0 0 1 4) 0 1 0 5) 1 0 0	1) 0 0 0 2) 0 0 0 3) 0 0 1 4) 0 1 0 5) 1 1 1	1) 0 0 0 2) 0 0 0 3) 0 0 1 4) 0 1 1 5) 1 1 0	1) 0 0 0 2) 0 0 1 3) 0 0 1 4) 0 1 0 5) 1 1 0

TABLE I (continued)

EXHAUSTIVE ENUMERATION OF 2 CUBED IN 5 RUNS

PARAMETER	7TH DESIGN	8TH DESIGN	9TH DESIGN	10TH DESIGN	11TH DESIGN
MEAN	0.437500	0.218750	0.218750	0.250000	0.375000
A1	0.437500	0.218750	0.218750	0.250000	0.500000
B1	0.250000	0.218750	0.218750	0.437500	0.500000
C1	0.250000	0.218750	0.218750	0.437500	0.875000
ESTIMATION INDEX	0.409600	0.819200	0.819200	0.409600	0.204800
FITTING INDEX	0.581818	0.914286	0.914286	0.581818	0.355556
N	5	5	5	5	5
DESIGNS	1) 0 0 0 2) 0 0 1 3) 0 1 0 4) 0 1 1 5) 1 0 0	1) 0 0 0 2) 0 0 0 3) 0 1 1 4) 1 0 1 5) 1 1 0	1) 0 0 0 2) 0 0 1 3) 0 1 0 4) 1 0 0 5) 1 1 1	1) 0 0 0 2) 0 0 1 3) 0 1 0 4) 1 0 1 5) 1 1 0	1) 0 0 1 2) 0 0 1 3) 0 1 0 4) 1 0 0 5) 1 1 0

3. Correspondence

The theory for mixed factorial designs is less well developed than that for designs in which all factors appear at the same number of levels. A useful technique is to construct a design with all factors at the same number of levels, then replace some of the factors with ones of real interest using a fixed correspondence between sets of levels. The best-known examples of this technique are the proportional-frequency designs of Addelman [4]. To demonstrate this approach consider a Graeco-Latin Square of side 3.

$$\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 1 & 1 & 1 \\
0 & 2 & 2 & 2 \\
1 & 0 & 1 & 2 \\
1 & 1 & 2 & 0 \\
1 & 2 & 0 & 1 \\
2 & 0 & 2 & 1 \\
2 & 1 & 0 & 2 \\
2 & 2 & 1 & 0
\end{array}$$

The last two factors may be replaced by two-level factors by using the correspondence

$$\begin{array}{l}
0 \rightarrow 0 \\
1 \rightarrow 1 \\
2 \rightarrow 1
\end{array} ,$$

which results in the design

0	0	0	0
0	1	1	1
0	2	1	1
1	0	1	1
1	1	1	0
1	2	0	1
2	0	1	1
2	1	0	1
2	2	1	0

This design is quite efficient, having a fitting index of .93 and an estimation index of .79. A number of different types of correspondences is given by Addelman in [4].

4. Permutation-Invariant Designs

The salient property of permutation-invariant designs, defined in [5], is that estimates involving factors which appear at the same number of levels have the same variance properties. More formally, the cross-product matrix X'X remains unaltered if factors appearing at the same number of levels are permuted. An example of a $3^2 \times 2^3$ main effect design, for which $I_F = .80$ and $I_E = .47$, is:

0	0	1	0	0
0	1	0	0	1
0	2	0	1	0
1	0	0	0	0
1	1	1	1	1
1	2	1	1	1
2	0	0	1	1
2	1	1	1	0
2	2	1	0	1

If one uses a standard parameterization, the X and X'X matrices for this design are:

$$X = \begin{bmatrix} 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 0 & 1 & -2 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & 0 & -1 & -2 & 1 & -1 & -1 & -1 \\ 1 & 0 & 0 & -2 & -2 & 1 & 1 & 1 \\ 1 & 0 & 1 & -2 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 0 & 1 & -2 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 \end{bmatrix}, \quad (X'X) = \begin{bmatrix} 9 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 6 & 0 & 0 & 0 & 2 & 2 & 2 \\ 0 & 0 & 6 & 0 & 0 & 2 & 2 & 2 \\ 0 & 0 & 0 & 18 & 0 & -2 & -2 & -2 \\ 0 & 0 & 0 & 0 & 18 & -2 & -2 & -2 \\ 1 & 2 & 2 & -2 & -2 & 9 & 1 & 1 \\ 1 & 2 & 2 & -2 & -2 & 1 & 9 & 1 \\ 1 & 2 & 2 & -2 & -2 & 1 & 1 & 9 \end{bmatrix}$$

Permutation of factors appearing at the same numbers of levels has the effect of permuting rows and columns of the submatrices in the partitioned cross-product matrix. Since the submatrices are invariant, the design is permutation-invariant.

This principle has been used* to construct a series of as yet unpublished saturated second-order designs for three-level factors. For five factors the design contains the treatment combination 0 0 0 0 0, the five treatment combinations which are permutations of 1 1 1 1 0, the five permutations of 2 2 2 2 0, and the ten permutations of 2 2 0 0 0. For this design the fitting index is .66 and the estimation index is 2.35. Relative to the full factorial but adjusting for the difference in the number of runs, the efficiency of the estimate of the mean is 82%, of the linear main effects is 114%, of the quadratic main effects is 25%, and of the linear by linear interactions is 171%. The reason that the linear effects and interactions are so efficient is that the points of the design tend to be concentrated around the outside of the hypercube.

*This work was carried out by R. L. Rechtschaffner of Rocketdyne's Statistical Test Design Unit.

5. Balancing Levels

A very useful technique for constructing designs is to start with an ordinary factorial structure for the first group of factors, and then insert the remaining factors in such a way that pairs of levels appear together with nearly equal frequencies. For example, the following two designs are obtained by adding another two-level factor to a basic 2x3 full factorial:

Design 1	Design 2
0 0 0	0 0 0
0 1 1	0 1 1
1 0 1	1 0 1
1 1 0	1 1 1
2 0 0	2 0 1
2 1 1	2 1 0

Their variance properties are given in Table II.

EXAMPLES

Three ad hoc designs which have been used successfully at Rocketdyne will be mentioned briefly. The first involved determination of char formation rate in ablative heat-shield material under simulated reentry conditions. The testing was done in a small stationary hydrogen-oxygen rocket engine. The experimental variables were rocket engine combustion chamber pressure, propellant mixture ratio, and the angle of the sample in the rocket exhaust. The experimental design chosen was one of the optimum 2^3 designs in 5 runs discussed earlier.

TABLE II

3x2x2 'BALANCED' DESIGNS

PARAMETER	1ST DESIGN	2ND DESIGN
MEAN	0.166667	0.194444
A1	0.250000	0.250000
A2	0.083333	0.111111
B1	0.187500	0.166667
C1	0.187500	0.250000
ESTIMATION INDEX	0.888889	0.666667
FITTING INDEX	0.952381	0.833333
N	6	6

Run Number	Target Chamber Pressure (Psia)	Target Mixture Ratio	Inclination Angle (degrees)
1	170	4	0
2	250	4	$12\frac{1}{2}$
3	170	16	$12\frac{1}{2}$
4	250	16	0
5	250	16	$12\frac{1}{2}$

Another such design was used on a Signal Corps battery program. The experimental work involved screening 4 cathode materials, 3 solvents, and 4 salts. The design was constructed by balancing the levels of the second four-level factor within the framework of the 12-run 3 x 4 factorial.

Run Number	Cathode	Solvent	Salt
1	0	0	0
2	0	1	1
3	0	2	3
4	1	0	1
5	1	1	0
6	1	2	2
7	2	0	2
8	2	1	3
9	2	2	1
10	3	0	3
11	3	1	2
12	3	2	0

Although there was no justification for assuming interactions did not exist, they could reasonably be expected to be less important than main effects. It was intended that this experiment be used to eliminate from contention some of the candidate materials with just a few tests, so that later tests could concentrate on the better ones. The actual decision made from these tests was that none of the four cathode materials was satisfactory, and later testing should be directed at finding additional materials. If all interactions had been considered, 48 tests, using these four unsatisfactory materials, would have been required.

The balancing technique was used effectively to construct a $3^4 \times 2^3$ design in 27 runs for a program concerned with the evaluation of fiber-reinforced plastic laminates. The variables are as follows:

Variable	Code	Levels
Bonding Pressure	A	3
Bonding Temperature	B	3
Resin Concentration	C	3
Post-Cure Temperature	D	3
Bonding Time	E	2
Post-Cure Time	F	2
Fiber Quality	G	2

It was established that the linear interactions AB, AC, BC, BE, and DF are expected to be important. Since the factor D does not interact with the other three three-level factors, the starting point was a 1/3 replicate of a 3^4 using as defining contrast $I = A^2 B^2 C^2 D$. For the 2^3 part of the design three replications of the 2^3 plus three additional points were used. The 2^3 part was associated with the 3^4 part a number of ways, and the best design selected. The third and fourth designs were singular. The first, and best, design is presently being implemented.

	DESIGN NUMBER 1	DESIGN NUMBER 2	DESIGN NUMBER 3	DESIGN NUMBER 4	DESIGN NUMBER 5
1)	0 0 0 0 0 0 0	0 0 0 0 0 0 0	0 0 0 0 0 0 0	0 0 0 0 0 0 0	0 0 0 0 0 0 0
2)	0 0 1 2 1 1 1	0 0 1 2 0 0 1	0 0 1 2 1 0 0	0 0 1 2 1 0 0	0 0 1 1 1 1 1
3)	0 0 2 1 0 0 0	0 0 2 1 1 1 0	0 0 2 1 0 1 0	0 0 2 1 0 1 0	0 0 2 2 1 0 0
4)	0 1 0 2 1 0 1	0 1 0 2 1 1 1	0 1 0 2 1 0 0	0 1 0 2 1 0 0	0 1 0 2 1 0 1
5)	0 1 1 1 0 0 1	0 1 1 1 0 0 1	0 1 1 1 1 1 0	0 1 1 1 1 1 0	0 1 1 0 0 0 1
6)	0 1 2 0 1 0 1	0 1 2 0 1 1 1	0 1 2 0 1 1 1	0 1 2 0 1 1 1	0 1 2 1 1 1 0
7)	0 2 0 1 1 1 0	0 2 0 1 0 0 0	0 2 0 1 0 1 0	0 2 0 1 0 1 0	0 2 0 1 1 1 1
8)	0 2 1 0 1 1 1	0 2 1 0 1 0 1	0 2 1 0 1 1 1	0 2 1 0 1 1 1	0 2 1 2 0 1 1
9)	0 2 2 2 0 1 0	0 2 2 2 0 1 0	0 2 2 2 0 0 1	0 2 2 2 0 0 1	0 2 2 0 0 1 0
10)	1 0 0 2 0 0 1	1 0 0 2 1 0 1	1 0 0 2 1 0 0	1 0 0 2 1 0 0	1 0 0 2 1 1 1
11)	1 0 1 1 0 0 1	1 0 1 1 0 1 1	1 0 1 1 1 1 0	1 0 1 1 1 1 0	1 0 1 0 0 1 1
12)	1 0 2 0 1 0 1	1 0 2 0 0 1 1	1 0 2 0 1 1 1	1 0 2 0 1 1 1	1 0 2 1 0 1 0
13)	1 1 0 1 0 1 1	1 1 0 1 0 0 1	1 1 0 1 1 1 0	1 1 0 1 1 1 0	1 1 0 1 0 0 0
14)	1 1 1 0 1 1 0	1 1 1 0 1 1 0	1 1 1 0 0 0 0	1 1 1 0 0 0 0	1 1 1 2 1 1 1
15)	1 1 2 2 0 1 0	1 1 2 2 1 0 0	1 1 2 2 1 0 1	1 1 2 2 1 0 1	1 1 2 0 1 0 0
16)	1 2 0 0 0 1 1	1 2 0 0 1 0 1	1 2 0 0 1 1 1	1 2 0 0 1 1 1	1 2 0 0 1 0 1
17)	1 2 1 2 1 0 0	1 2 1 2 0 1 0	1 2 1 2 1 0 1	1 2 1 2 1 0 1	1 2 1 1 0 0 1
18)	1 2 2 1 0 0 0	1 2 2 1 0 1 1	1 2 2 1 0 1 1	1 2 2 1 0 1 1	1 2 2 2 1 1 0
19)	2 0 0 1 1 1 0	2 0 0 1 1 1 0	2 0 0 1 0 1 0	2 0 0 1 0 1 0	2 0 0 1 1 0 1
20)	2 0 1 0 1 1 1	2 0 1 0 0 1 1	2 0 1 0 1 1 1	2 0 1 0 1 1 1	2 0 1 2 0 0 1
21)	2 0 2 2 0 1 0	2 0 2 2 1 1 0	2 0 2 2 0 0 1	2 0 2 2 0 0 1	2 0 2 0 1 1 0
22)	2 1 0 0 0 1 1	2 1 0 0 1 1 1	2 1 0 0 1 1 1	2 1 0 0 1 1 1	2 1 0 0 1 1 1
23)	2 1 1 2 1 0 0	2 1 1 2 1 0 0	2 1 1 2 1 0 1	2 1 1 2 1 0 1	2 1 1 1 0 1 1
24)	2 1 2 1 0 1 1	2 1 2 1 1 0 0	2 1 2 1 0 1 1	2 1 2 1 0 1 1	2 1 2 2 0 1 0
25)	2 2 0 2 1 1 0	2 2 0 2 0 1 0	2 2 0 2 0 0 1	2 2 0 2 0 0 1	2 2 0 2 0 0 0
26)	2 2 1 1 1 0 0	2 2 1 1 0 0 0	2 2 1 1 0 1 1	2 2 1 1 0 1 1	2 2 1 0 1 1 1
27)	2 2 2 0 1 0 1	2 2 2 0 1 0 1	2 2 2 0 0 0 0	2 2 2 0 0 0 0	2 2 2 1 1 0 0

3X3X3X3X2X2X2 IN 27 RUNS.

PARAMETER	1ST DESIGN	2ND DESIGN	3RD DESIGN	4TH DESIGN	5TH DESIGN
MEAN	0.040023	0.038683	***********	***********	0.039227
A1	0.065645	0.066797	0.101365	0.101365	0.060946
A2	0.023191	0.021691	0.045917	0.045917	0.024405
B1	0.068331	0.144732	0.101365	0.101365	0.0[illegible]7834
B2	0.021630	0.033605	0.043643	0.043643	0.019680
C1	0.101666	0.071088	0.101365	0.101365	0.[illegible]6720
C2	0.030675	0.026362	0.045917	0.045917	0.1009[illegible]6
D1	0.068076	0.136054	***********	***********	0.060441
D2	0.021945	0.034868	***********	***********	0.013519
E1	0.065291	0.067670	0.535088	0.535088	0.081[illegible]71
F1	0.077900	0.094148	***********	***********	0.046593
G1	0.052820	0.071160	0.367325	0.367325	0.293654
A1B1	0.147604	0.095345	0.186404	0.186404	0.1[illegible]77[illegible]1
A1C1	0.095526	0.146515	0.175439	0.175439	0.115[illegible]74
B1C1	0.102529	0.089120	0.186404	0.186404	0.093785
B1E1	0.090778	0.287987	0.078947	0.078947	0.080452
D1F1	0.139308	0.166098	***********	***********	0.094064
ESTIMATION INDEX	0.070734	0.022297	0.000000	0.000000	0.036923
FITTING INDEX	0.669524	0.510378	0.000000	0.000000	0.480730
N	27	27	[illegible]	27	27

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NON-ORTHOGONAL DESIGNS OF EVEN RESOLUTION

INTRODUCTION AND SUMMARY

Incomplete factorial designs for estimating all main effects or all main effects and all two-factor interactions have received considerable treatment in the literature. An intermediate category, which has received much less attention, contains designs from which the main effects can be estimated unbiased by two-factor interactions, but the interactions themselves cannot be estimated. Such designs, said to be of resolution 4, are the most important of the designs of even resolution, and consequently receive the most attention in this paper.

Within the more restricted class of fractional factorials, properties and construction technique for designs of all resolution numbers are well known. Such designs may be constructed immediately from a defining contrast, in which case the resolution is equal to the minimum number of letters in the elements of this contrast. An effect of order q ($q = 0$ for the grand mean, $q = 1$ for main effects, etc.) in a fractional factorial design of resolution r has as aliases terms of order $r - q$ and higher.

Outside of the family of fractional factorials, as one might expect, the situation is not as straightforward. The following definition of resolution for such designs was provided in [1]: a design of odd resolution r is such that all effects through order $\frac{1}{2}(r-1)$ are estimable ignoring higher order terms; a design of even resolution r is such that effects of order $\frac{1}{2}(r-2)$ or lower are estimable ignoring those of order $\frac{1}{2}(r+2)$ or higher. For design of even resolution those effects of order $\frac{1}{2}r$ are not estimable but do not appear as aliases of those which are.

The analysis of designs of odd resolution is straightforward. The ordinary least-squares technique is used to estimate β, the vector of parameters. Letting $EY = X\beta$, where Y is the vector of responses from a design, we have $\hat{\beta} = (X'X)^{-1}X'Y$, and $\operatorname{Var} \hat{\beta} = (X'X)^{-1}\sigma^2$. A design is of the required resolution if and only if the corresponding cross-product matrix $X'X$ is nonsingular. A necessary condition is that the number of runs N be at least as large as the number of parameters.

This paper reviews previous work on designs of even resolution. The estimation theory for such designs is developed. It is proved that a 2^n design of resolution 4 contains at least $2n$ runs. The method of proof gives insight into the structure of minimal designs of resolution 4, and leads to a characterization of resolution 4 designs. The "foldover principle," due to Box and Wilson [2], is discussed in detail, and it is shown that this principle may be used to generate minimal designs of resolution 4. It is conjectured that the only minimal designs of resolution 4 are foldover designs. Designs of resolution 2 and 6 are discussed briefly.

PREVIOUS WORK

References to fractional factorials of even resolution are scattered throughout the standard literature (for example, [3], and [4]). The first comprehensive treatment of such designs was given by Box and Hunter [5], who introduced the term "resolution." They showed that eight factors could be accommodated in 16 runs, twelve in 24 runs, and in general $4k$ factors in $8k$ runs. The designs are constructed by the "foldover" principle from saturated resolution 3 (Plackett-Burman) designs which exist if the number of factors is of the form $4k-1$ for $k \leq 25$ [6]. This principle can best be described by means of the design matrix for a Plackett-Burman design; for example, consider the 2^3 in 4 runs:

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} .$$

The "mirror" image of this matrix is formed by interchanging 0 and 1; in the example we have:

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} .$$

The completed foldover design consists of the original design and its "image" as submatrices, augmented by a new factor at its high level in the first half and its low level in the second. In the example being considered, the complete 2^4 resolution 4 design in 8 runs is

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Box and Wilson [2] provide a proof that the foldover procedure yields designs with the property that first-order effects (i.e., main effects) have no second-order effects (interactions) as aliases. Although this is proved in the context of response surface experiments, it is equally valid for incomplete factorials and is proved in this context in a subsequent section. An even simpler proof is available if the initial design is a fractional factorial. For the first half of the design the defining contrast contains the first factor A plus additional terms none of which has fewer than three letters. In the second half the alias structure is the same, except that all elements of the defining contrast with an odd number of letters have their sign changed. The defining contrast of the entire design, obtained by adding those of the subdesigns, contains only terms containing an even number of letters, all with four or more. In the present example the defining contrasts are I = A = -BCD = -ABCD and I = -A = BCD = -ABCD for the subdesigns and I = -ABCD for the whole.

An alternative procedure for constructing fractional factorials of resolution 4 is also given by Box and Hunter. Starting from a full factorial involving a subset of the factors, new factors are included by equating them to interactions involving an odd number of the original factors. For example, to a complete 2^4 can be added $E = ABC$, $F = ABD$, $G = ACD$, and $H = BCD$, to complete the eight-factor 16-run resolution 4 design.

Recent unpublished work by Cuthbert Daniel [7] motivated me to initiate the study which resulted in this paper. He showed that non-orthogonal resolution 4 designs exist and gave minimal designs for 3 factors in six runs and for 5 factors in 10 runs. Scrutiny of Daniel's designs reveals that they may be considered as having been constructed from minimal resolution 3 designs by the foldover technique.

ESTIMATION IN EVEN-RESOLUTION DESIGNS

Ordinarily from a model of the form $EY = X\beta$ one can obtain the least-squares estimate of β, which is given by $\hat{\beta} = (X'X)^{-1} X'Y$. In even-resolution designs the matrix $X'X$, however, is singular so that this procedure is not applicable. Let the model be rewritten in the form $EY = X_1\beta_1 + X_2\beta_2 + X_3\beta_3$, where Y is the $N \times 1$ vector of responses, β_1 is the $p \times 1$ vector of parameters to be estimated, and β_2 and β_3 are respectively $q \times 1$ and $r \times 1$ vectors of parameters which are not to be estimated. Furthermore, let the selection of the parameters in the vector β_2 be such that the matrix $[X_1, X_2]$ is of full rank $p + q$. Since this matrix is of full rank, there must exist matrices H_1 and H_2 such that X_3 can be expressed in the form $X_3 = X_1H_1 + X_2H_2$. From the requirement that the design be of even resolution it can be shown that the matrix H_1 must be zero. Let $\hat{\beta}_1$ be given by $J\,Y$. We have $E\,\hat{\beta}_1 = \beta_1$ which can be rewritten

$$E\,JY = J\,(X_1\beta_1 + X_2\beta_2 + X_3\beta_3) = \beta_1 .$$

Therefore we must have $JX_1 = I$, $JX_2 = 0$, and $JX_3 = 0$. But $JX_3 = JX_1H_1 + JX_2H_2 = IH_1 + 0H_2 = H_1$, so that H_1 must be the zero matrix.

Analysis of even resolution designs can be facilitated by an appropriate partitioning of the unestimated parameters into β_2 and β_3. Let $X'X$ be written in the form

$$X'X = \begin{bmatrix} A & B & D \\ B' & C & F \\ D' & F' & G \end{bmatrix}$$

where the partitioning corresponds to that of X into X_1, X_2, and X_3. The normal equations may now be expressed in the form

$$A\,\hat{\beta}_1 + B\,\hat{\beta}_2 + D\,\hat{\beta}_3 = X_1'\,Y$$

$$B'\hat{\beta}_1 + C\,\hat{\beta}_2 + F\,\hat{\beta}_3 = X_2'\,Y$$

$$D'\hat{\beta}_1 + F'\hat{\beta}_2 + G\,\hat{\beta}_3 = X_3'\,Y\ .$$

By the assumptions made previously, the matrix $\begin{bmatrix} A & B \\ B' & C \end{bmatrix}$ is nonsingular; let its inverse be given by $\begin{bmatrix} U & V \\ V' & W \end{bmatrix}$. By the usual rules for inverting partitioned matrices we have

$$U = (A - BC^{-1} B')^{-1}$$
$$V = -U B C^{-1}$$
$$W = C^{-1} - C^{-1} B' V.$$

A particular solution to the normal equations is given by

$$\hat{\beta}_1 = U X_1' Y + V X_2' Y$$
$$\hat{\beta}_2 = V' X_1' Y + W X_2' Y$$
$$\hat{\beta}_3 = 0.$$

This may easily be verified by substituting this solution back into the normal equations. By the definition of estimability of β_1, every solution of the normal equations has the same value for $\hat{\beta}_1$; that is, its value is independent of the way in which the unestimated parameters are partitioned into β_2 and β_3.

MINIMAL RESOLUTION 4 DESIGNS

The development in the last section can be used in proving that the smallest resolution 4 designs for n factors must contain at least $2n$ runs. The proof is accomplished by showing that certain interaction parameters must be in the vector β_2 since under the assumption that $\beta_3 = 0$, β_1 and β_2 are jointly estimable.

THEOREM 1*.

A resolution 4 design for n factors at two levels must contain at least $2n$ runs.

*Barry Margolin, Harvard, independently developed an identical proof for this theorem.

PROOF.

Let $X_1, \ldots, X_n$ be the column vectors of the matrix X associated with the n main effects. Let $Z_1, \ldots, Z_n$ represent the column vectors associated with the grand mean and the interactions of the first factor with the second, third, ..., n-th, in that order. Note that z_{ij}, the i-th component of Z_j, is given by $z_{ij} = x_{i1} x_{ij}$, where x_{ij} is the i-th component of X_j. Since main effects are estimable, $X_1, \ldots, X_n$ are linearly independent. Because of the nature of the Z_j's it follows that the Z_j's are also mutually independent. It will now be shown that the requirement that the design be of resolution 4 implies that the X's and Z's are also independent of one another.

Suppose the design contains $N < 2n$ runs. Select any vectors $W_1, \ldots, W_{N-n}$ such that $[X_1, \ldots, X_n, W_1, \ldots, W_{N-n}]$ is of full rank N. Since the design is of resolution 4 all the Z's are expressible in the form $Z = XH_1 + WH_2$, using the obvious definitions of the matrices Z, X, and W. Since the matrix H_1 must be equal to 0, $Z = WH_2$; but there are more linearly independent Z's than W's, which is a contradiction.

Essentially the same proof can be used to give a characterization of resolution 4 designs.

THEOREM 2.

In addition to the main effects, the grand mean and all two-factor interactions involving a given factor can be estimated from a resolution 4 design under the assumption that the remaining interactions are zero. Conversely, if it is true that for each choice of a single factor all two-factor interactions involving it, the grand mean, and main effects are estimable ignoring the remaining interactions, then the design is of resolution 4.

PROOF.

In the preceding proof it was shown that in any resolution 4 design the vectors $[X_1, \ldots, X_n, Z_1, \ldots, Z_n]$ are mutually linearly independent. Since the designation of which factor was used to define the Z's was arbitrary, the first part of this theorem follows.

To prove the converse, let $Z_1^{(1)}, \ldots, Z_n^{(1)}$ be the column vectors associated with the grand mean and two-factor interactions involving the first factor; $Z_1^{(2)}, \ldots, Z_n^{(2)}$ be associated with the grand mean and two-factor interactions involving the second factor; $\ldots$; $Z_1^{(n)}, \ldots, Z_n^{(n)}$ be associated with the grand mean and two-factor interactions involving the n-th factor. The hypothesis is that for each choice i the vectors $[X_1, \ldots, X_n, Z_1^{(i)}, \ldots, Z_n^{(i)}]$ are mutually linearly independent. Therefore the space spanned by the set

$[Z_1^{(1)}, \ldots, Z_n^{(1)}, \ldots, Z_1^{(n)}, \ldots, Z_n^{(n)}]$ is independent of that spanned by the X's. Select any basis for the former subspace and assign the corresponding parameters to the vector β_2. The columns for the remaining parameters are all expressible as linear combinations of those in the basis, so that the matrix H_1 is zero, which in turn implies that the design is of resolution 4.

Although the characterization of resolution 4 designs provided by this theorem is not particularly useful for verifying whether or not a given design is of resolution 4, it does have the following corollary.

COROLLARY.

Augmenting a design of even resolution by additional treatment combinations does not reduce the resolution number.

Although this corollary appears trivially obvious, a direct proof without using Theorem 2 is frustratingly involved.

THE FOLDOVER PRINCIPLE

The foldover principle, described above, can be used to generate a wide variety of designs of even resolution. If a design is of resolution 3, the foldover design made from it is of resolution 4. A proof in the context of 2^n designs is as follows:

Suppose U is the coefficient matrix for a resolution 3 design. The coefficient matrix for the foldover design is of the form

$$X = \begin{bmatrix} e & U & V \\ e & -U & V \end{bmatrix},$$

where e is an appropriately dimensioned vector of 1's. The coefficient vectors for the main effects are in the U part of the partitioned matrix, and those for two-factor interactions are in the V part. The negative of appears in the second half of the design by definition of the foldover principle. In the first half, each element of a column of V is the product of the corresponding elements in two columns of U; in the second half, the matrix V is duplicated since the negative of each column of U is involved. The cross-product matrix is

$$X'X = \begin{bmatrix} 2\, e'e & 0 & 2\, e'V \\ 0 & 2\, U'U & 0 \\ 2\, V'e & 0 & 2\, V'V \end{bmatrix}.$$

Since the main-effect part $2U'U$ of this matrix is nonsingular and orthogonal to the remainder, the design is in fact of resolution 4. Thus, for foldover designs the subspace spanned by the columns associated with the main effects (the vectors $X_1, \ldots, X_n$ in the notation of the previous section) is not only independent of but also orthogonal to the subspace spanned by the remaining columns (the vectors $Z_1^{(1)}, \ldots, Z_n^{(1)}, \ldots, Z_n^{(n)}$).

The foldover technique may be employed on n-run, (n-1)-factor designs of resolution 3 to yield 2n-run, n-factor designs of resolution 4. By Theorem 1, such designs will be the smallest possible designs for this experimental situation. Designs which are minimal and which appear to be among the most efficient possible are given below. Only half the treatment combinations are given for each design, the other half being obtained by "multiplying" in the usual fashion each of the listed treatment combinations by the treatment combination with all factors at their high level. The first design is due to Daniel [7]. Fractional factorials are available for 4 and 8 factors. In the column labeled "variance" is given the multiple of σ^2 giving the variance of each main-effect estimator.

Number of Factors	Number of runs	Variance	Runs in Half of Design
3	6	1/4	a, b, c
5	10	1/9	a, b, c, d, e
6	12	1/10	ab, ac, bc, d, e, f
7	14	11/100	a, b, c, d, e, f, g

Based on the work to date with non-orthogonal designs of resolution 4, the following conjecture is made.

CONJECTURE.

Foldover designs form a complete class of minimal 2^n designs of resolution 4. That is, there exist no resolution 4 designs with $2n$ runs and n factors except those constructed by the foldover technique.

The conjecture has been proved for $n = 2$, 3, and 4. For the case of two factors the only resolution 4 design is the full factorial, which is itself a foldover design. For three factors it is relatively easy to enumerate all possible six-run designs and note that the only designs of resolution 4 are foldover designs. For the case of four factors a proof that the only resolution 4 designs are foldover designs has been constructed. In order to prove this result, consider the submatrix consisting of the columns of X associated with the parameters I, AB, AC, and AD. There are eight possible combinations of values for the elements in the rows of this submatrix. In the X matrix the elements of the columns of X associated with BC are simply the product of the elements in the columns AB and AC. If a design is of resolution 4 then the elements of BC must also be linear combinations of the elements of the four columns I, AB, AC, and AD. Under these restrictions only four of the eight possible combinations of values for AB, AC, and AD may appear in the design. This fact in turn implies that the design must be a foldover design.

DESIGNS OF OTHER RESOLUTION NUMBERS

A design of resolution 2 is such that an estimate of the grand mean is available which is unbiased by main effects. For any number of factors, such a design is provided by any two runs which are complementary, in the sense that each factor appears at its high level in one and at its low level in the other. The variance of the estimated grand mean is $\frac{1}{2}\sigma^2$ using any such design. Such designs are the only minimal designs of resolution 2, and may be considered as foldover designs.

Fractional factorials of resolution 6 may be constructed by the foldover principle from fractional factorials of resolution 5. The argument involving defining contrasts given in an earlier section for designs of resolution 4 is easily extended to encompass this situation. Indeed, the foldover principle can be used to construct a design of any even resolution number from a fractional factorial of the next lower (odd) resolution number. The resulting designs are, of course, also fractional factorials.

The foldover principle may be applied to more general designs of resolution 5, but the result need not satisfy the definition of a design of resolution 6 given in the first section of this paper. Let the coefficient matrix for a foldover design constructed from a resolution 5 design be represented by

$$X = \begin{bmatrix} e & U & V & W \\ e & -U & V & -W \end{bmatrix}$$

Here the U part corresponds to main effects, V to two-factor interaction, and W to three-factor interactions. The cross-product matrix is

$$X'X = \begin{bmatrix} 2\, e'e & 0 & 2\, e'v & 0 \\ 0 & 2\, U'U & 0 & 2\, U'W \\ 2\, V'e & 0 & 2\, V'V & 0 \\ 0 & 2\, W'U & 0 & 2\, W'W \end{bmatrix}.$$

It is clear that estimates of the grand mean and of the two-factor interactions are available which are unbiased by three-factor interactions. The estimates of the main effects will in general, however, have three-factor interactions as aliases. In order not to have such aliasing, the columns of W must be linearly independent of those for U.

Outside the class of fractional factorials nothing appears to be known about designs which are truly of resolution 6 (that is, for which both two-factor interactions and main-effects have no three-factor interactions as aliases). An argument analogous to Theorem 1 can be used to show that the minimum number of runs in such a design is $1 + \binom{n}{1}+\binom{n}{2}+ \binom{n-1}{2} = n^2-n+2$. For three factors the only design of resolution 6 is the full factorial (which is of resolution 7). For four factors there is available a 15-run design of resolution 7, but there does not seem to be a 14-run design of resolution 6. It is not known whether there exists a five-factor design of resolution six containing between 22 runs, the minimum by the above formula, and 26 runs, the minimum number for a resolution 7 design. For the case of six factors, the half-replicate is a minimal resolution 6 design.

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SATURATED SEQUENTIAL FACTORIAL DESIGNS

INTRODUCTION AND SUMMARY

In the early phases of an experimental investigation, the experimenter may be unaware or have only a general idea of some of the variables which have important influences on the important responses. Typically he will reject the apparent rigidity of a formal statistical test plan and do exploratory experimentation. The result of such experimentation may well be a sequence of runs each of which introduce a new variable or a new level for an old variable.

It has become axiomatic in the statistical experimental design literature to discourage the practice of varying one factor at a time. For the case of factors each at two levels, an excellent exposition of the statistical arguments against such designs was given by Fisher in The Design of Experiments, Sections 37 and 38 [1]. He bases his attack on the fact that the variances of the main-effect estimates using such designs are considerably larger than with orthogonal designs, and on their lack of information about interactions.

On the other hand, the experimenter often likes such designs because he finds out more rapidly whether a new factor has any effect. He continually receives information rather than having to wait till the entire experiment is completed. If the magnitudes of the effects he is interested in are several times as large as experimental error, if he does not need to describe these effects precisely, and if there are no interactions, there is no particular disadvantage in experimenting in this way. Cuthbert Daniel [2] has presented these positive aspects of such designs, and pointed out that they can often be augmented to form a half replicate plus one additional run, in which case the lost efficiency is for the most part regained.

In an earlier paper [3] I introduced the concept of contractible designs, which have the property that much of the information in the experiment will be available even if the experiment is prematurely halted or the course of the experiment is significantly altered. One-at-a-time designs represent an extreme class of contractible designs, in that some information is available no matter when the experiment is terminated.

The first few sections of this paper develop a theory for one-at-a-time designs for estimating the main effects of two-level factors. It is shown that $\frac{1}{2}\sigma^2$ is a lower bound for the variance of a main-effect estimate from a saturated one-at-a-time design. (This result was previously given in [4].) A characterization of designs for which the lower bound is achieved is presented. The results on two-level factors are extended to the case in which there is no restriction on the numbers of levels for the factors. Situations may arise in which the factors can safely be introduced in small sets, rather than one at a time. Details are derived for block sizes of 2, 3, and 4. Finally, inclusion of interaction terms in the model is considered. It is shown that the estimates of main effects of factors involved in interactions are improved.

VARIANCE BOUNDS FOR ONE-AT-A-TIME DESIGNS FOR TWO-LEVEL FACTORS

The first run of a one-at-a-time design has all factors at their initial levels, which for convenience will be considered the low levels, denoted by 0 or -1. Each successive run introduces the high level, denoted by 1 or +1, of one of the factors. The factors will be considered as being ordered in such a way that the <u>i</u>th factor first appears at its high level in the <u>(i+1)</u>st run. After a factor has been introduced (i.e., after it appears for the first time at its high level) it may stay at its high level, revert to its low level, or be varied between its two levels on subsequent tests. Thus there is a wide latitude of possible one-at-a-time designs.

Experiments for estimating the main effects of two-level factors are conventionally analyzed in terms of the coefficient matrix X as follows. The first column of X corresponds to the grand mean and has all its components equal to 1. Each of the remaining columns corresponds to one of the factors, and each row corresponds to a run. According to whether a given factor is at its high or low level in a given run, the corresponding element of X contains the entry +1 or -1.

Suppose a vector Y of N responses is obtained from the experiment. Under the assumption that there are no interactions we may write $Y = X\beta + e$, where β is the vector of the unknown parameters and e is a vector of independent random errors having mean zero and common variance σ^2. The least-squares estimate $\hat{\beta}$ of β is $\hat{\beta} = (X'X)^{-1}X'Y$. The covariance matrix of $\hat{\beta}$ is $\sigma^2(X'X)^{-1}$.

In addition to working with the traditional coefficient matrix X, it will be convenient to introduce a reduced matrix R. Where X has an element 1, R also has 1; where X has a -1, R has a zero. It may be verified that X and R are related through the triangular transformation matrix T according to the equation $X = RT$, as in the following example:

$$\begin{bmatrix} 1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & -1 & -1 & -1 & -1 & -1 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix} .$$

In general, t_{ij} is given by the following rules:

$t_{11} = 1$

$t_{1j} = -1 \; (j = 2, \ldots, n + 1)$

$t_{jj} = 2 \; (j = 2, \ldots, n+1)$

$t_{ij} = 0$ (otherwise).

It may be verified that T^{-1} has the following form

$$T^{-1} = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} \\ 0 & \frac{1}{2} & 0 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & & & \\ \cdot & \cdot & \cdot & \cdot & & \cdot & & \\ \cdot & \cdot & \cdot & \cdot & & & \cdot & \\ 0 & 0 & 0 & 0 & & & & \frac{1}{2} \end{bmatrix} .$$

If R is the reduced coefficient matrix for a one-at-a-time design, then (a) the first column of R consists solely of 1's; (b) the main diagonal of R consists of 1's, since the $\underline{i}$th factor appears at its high level in the $(\underline{i+1})$st run; and (c) the elements above the main diagonal are all 0, since the $\underline{i}$th factor remains at 0 until the $(\underline{i+1})$st run. Since R is lower triangular and has 1's down the main diagonal, the determinant of R is unity. Since the elements of R are integers any minor is integral. Since the elements of an inverse are by definition an appropriate minor divided by the determinant of the original matrix, R^{-1} also consists of integers. It follows from the form of T^{-1} that each element of $X^{-1} = T^{-1}R^{-1}$ must be a multiple of $\frac{1}{2}$.

THEOREM 1. For a one-at-a-time design containing $n+1$ runs and n factors at two levels, a lower bound for the variance of any estimate is $\frac{1}{2}\sigma^2$.

PROOF. The variances of the estimates are σ^2 times the diagonal elements of $(X'X)^{-1}$. Because X is square $(X'X)^{-1}$ reduces to $(X^{-1})(X^{-1})'$. The diagonal elements are therefore the sums of squares of the elements in each row of X^{-1}. We know already that the elements of X^{-1} are all multiples of $\frac{1}{2}$. The sum of squares of the elements in a row must therefore be a positive multiple of $\frac{1}{4}$. If the value were $\frac{1}{4}$, then all the elements would be zero except one which was equal to $\pm\frac{1}{2}$. The inner product of a row of X^{-1} and a column of X must of course be either 0 or 1. Since the elements of X are all either $+1$ or -1, the inner product of any column of X with a row containing a single $\frac{1}{2}$ would be $\pm\frac{1}{2}$. Therefore a lower bound to the sum of squares of elements of any row of X^{-1} is $\frac{1}{4}$, and the theorem is proved.

CHARACTERIZATION OF OPTIMUM ONE-AT-A-TIME DESIGNS

The most familiar family of one-at-a-time designs are those in which each factor returns to its low level after it has first been introduced. The general form of the matrices R, R^{-1}, and X^{-1} in this family are exemplified by the following five-factor case:

$$R = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} ; \quad R^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} ; \quad X^{-1} = \begin{bmatrix} -1\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & \\ -\frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & \\ -\frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} .$$

It will be noted that the variance of each main-effect estimates is $\frac{1}{2}\sigma^2$, the theoretical lower bound. The variance of the grand mean is $\sigma^2(n^2-3n+4)/4$ for the n-factor case.

It is of interest to inquire whether or not there is a family of designs in which the variance of the grand mean is also at the minimum level of $\frac{1}{2}\sigma^2$. The family of designs in which each factor is maintained at its high level satisfies this requirement. Again using a five-factor example to illustrate the general case, R, R^{-1}, and X^{-1} are as follows:

$$R = \begin{bmatrix} 1&0&0&0&0&0 \\ 1&1&0&0&0&0 \\ 1&1&1&0&0&0 \\ 1&1&1&1&0&0 \\ 1&1&1&1&1&0 \\ 1&1&1&1&1&1 \end{bmatrix} ; \quad R^{-1} = \begin{bmatrix} 1&0&0&0&0&0 \\ -1&1&0&0&0&0 \\ 0&-1&1&0&0&0 \\ 0&0&-1&1&0&0 \\ 0&0&0&-1&1&0 \\ 0&0&0&0&-1&1 \end{bmatrix} \quad X^{-1} = \begin{bmatrix} \frac{1}{2}&0&0&0&0&\frac{1}{2} \\ -\frac{1}{2}&\frac{1}{2}&0&0&0&0 \\ 0&-\frac{1}{2}&\frac{1}{2}&0&0&0 \\ 0&0&-\frac{1}{2}&\frac{1}{2}&0&0 \\ 0&0&0&-\frac{1}{2}&\frac{1}{2}&0 \\ 0&0&0&0&-\frac{1}{2}&\frac{1}{2} \end{bmatrix}$$

These two classes of designs are two extremes in which all factors are either returned to their initial level or are held at their new level. Both classes are special cases of a more general class of one-at-a-time designs, all of which have variances of $\frac{1}{2}\sigma^2$ for all the main-effect estimates. This class consists of designs in which for every $k \geq 2$ the $\underline{k}$th run differs from some previous run, say the ℓ_kth, only in the level of the $(\underline{k-1})$st factor. The estimate of the effect of the $(\underline{k-1})$st factor is $\frac{1}{2}$ times the $\underline{k}$th response minus the ℓ_kth. For the former of the two classes previously discussed $\ell_k \equiv 1$ and for the latter $\ell_k \equiv k$. This heuristic argument will now be formalized.

THEOREM 2. In a one-at-a-time design the variance of the main effect of a two-level factor achieves the lower bound of $\frac{1}{2}\sigma^2$ if and only if the run in which that factor is introduced differs from some previous run only in the level of that factor.

PROOF. The variance of the estimate of the effect of the $(\underline{k-1})$st factor will be $\frac{1}{2}\sigma^2$ if an only if the $\underline{k}$th row of $S \equiv R^{-1}$ contains a single nonzero off-diagonal element, which must be equal to -1. Assume that the $\underline{k}$th row of S is of this form and that the single element equal to -1 appears in the ℓth column $(\ell < k)$. Thus we have $s_{k\ell} = 1$, $s_{kk} = 1$, and $s_{kj} = 0$ for $j \neq \ell$ and $j \neq k$. Formal multiplication of the $\underline{k}$th row of S by the matrix $R = S^{-1}$ yields the system of equations $\Sigma_{m=1}^{n} s_{km} r_{mj} = \delta_{kj}$, which reduces to $-r_{\ell j} + r_{kj} = \delta_{kj}$, where δ_{kj} is the Kronecker δ. It follows that the $\underline{\ell}$th and $\underline{k}$th rows of R are identical except for the value corresponding to the level of the $(\underline{k-1})$st factor.

Now assume that the ℓth and kth rows of R are identical except that $r_{\ell k} = 0$ and $r_{kk} = 1$. Formal multiplication of the ℓth rows of R by the columns of S yields the two systems of equations $\Sigma_{m=1}^{n} r_{\ell m} s_{mj} = \delta_{\ell j}$ and $\Sigma_{m=1}^{n} r_{km} s_{mj} = \delta_{kj}$. Substraction of the former from the latter yields $\Sigma_{m=1}^{n} (r_{km} - r_{\ell m}) s_{mj} = s_{kj} = \delta_{kj} - \delta_{\ell j}$, or $s_{kk} = 1$, $s_{k\ell} = -1$, and $s_{kj} = 0$ for $j = k$ and $j = \ell$. The proof is now complete.

Often an experimenter may prefer to determine which level of each factor is better, and conduct the remaining experiments at the more desirable level. Thus, in general after a factor is introduced it will either be held at its high level or be returned to its low level for the remainder of the experiment. It can be verified that for this type of design the conditions of Theorem 2 are satisfied, and the lower bound is achieved for each main-effect estimate.

In the kind of experiments in which a one-at-a-time design might be useful, there may or may not be interest in obtaining a good estimate for the grand mean. The variance of the estimate of the grand mean will achieve the lower bound in a saturated design only if the treatment combination with all factor at their high levels is in the design. The only one-at-a-time series that can have this property is the one in which all factors remain at their high levels.

ONE-AT-A-TIME DESIGNS FOR MULTIPLE-LEVEL FACTORS

The results for two-level factors can be extended to the case in which each factor may have more than two levels fairly easily by a proper choice of parameterization. For a factor with m levels there are $m-1$ parameters necessary to describe its response. These main-effect parameters are defined as contrasts among the expected responses at the levels. Let the levels be designated by $\mu_1, \mu_2, \ldots, \mu_m$; then the parameterization will be $\beta_1 = \frac{1}{2}(\mu_2 - \mu_1)$, $\beta_2 = \frac{1}{2}(\mu_3 - \mu_1), \ldots, \beta_{m-1} = \frac{1}{2}(\mu_m - \mu_1)$. For an appropriate definition of the grand mean, the coefficient matrix X associated with this parameterization takes the form of the X matrix for a one-at-a-time design for $m-1$ two-level factors. Consider one five-level factor. The design with one run at each level has the X matrix

$$X = \begin{bmatrix} 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 \end{bmatrix} .$$

It is apparant that this is identical to the coefficient matrix for a one-at-a-time design for 4 two-level factors.

In many practical situation an experimenter may be interested in comparisons other than binary comparisons between the levels. For example, it may be natural to use as parameters for a five-level factor (a) a comparison of the average response at the first two levels with the average response at the last three levels, (b) an intercomparison of the first two levels, and (c) two intercomparisons of the last three levels. Given any such specific parameterization, a theorem analogous to Theorem 3 below can probably be proved. In order to avoid a commitment to a specialized parameterization, the theorem is given for simple binary comparisons only. Other parameterizations can be studied by resolving them into simple binary comparisons.

THEOREM 3. Suppose it is of interest to estimate $\frac{1}{2}$ the difference between the expected responses at any pair of levels for each multi-level factor. Then a lower bound for the variance of such an estimate obtained from a fully saturated one-at-a-time design is $\frac{1}{2}\sigma^2$.

PROOF. By convention let the first level of each factor be the one used in the first run. In the proof of Theorem 1 it was shown that the minimum sum of squares of a row of X^{-1} is achieved when the row has two nonzero entries, each having absolute value $\frac{1}{2}$. This suffices to prove that $\frac{1}{2}\sigma^2$ is the lower bound for the variance of a comparison of any level with the first. A comparison of any other two levels μ_i and μ_j is the difference of two comparisons $\beta_i = \frac{1}{2}(\mu_i - \mu_1)$ and $\beta_j = \frac{1}{2}(\mu_j - \mu_1)$. The variance of the difference $\hat{\beta}_i - \hat{\beta}_j$ is the sum of the variances minus twice the covariance. Since the rows of X^{-1} are by definition orthogonal to the first column of X the sum of the elements of any row of X^{-1}, except the first, is zero. Since the elements of X^{-1} are multiples of $\frac{1}{2}$, it follows that each row, in a sense, contains an even number of $\frac{1}{2}$'s. The variances of $\hat{\beta}_i$ and $\hat{\beta}_j$ are therefore multiples of $\frac{1}{2}\sigma^2$. Similarly, the covariances between $\hat{\beta}_i$ and $\hat{\beta}_j$, the sum of cross products of the corresponding rows of X^{-1}, are multiples of $\sigma^2/4$. It follows that $V(\hat{\beta}_i) + V(\hat{\beta}_j) - 2C(\hat{\beta}_i, \hat{\beta}_j)$ must be a multiple of $\frac{1}{2}\sigma^2$. We have now shown that the variance of $\frac{1}{2}$ the difference between the expected responses at any pair of levels is a multiple of $\frac{1}{2}\sigma^2$, so that the minimum value is $\frac{1}{2}\sigma^2$, which completes the proof.

Theorem 2 once again can be used to characterize the class of designs for which the bound is attained. In particular, the practice of maintaining the best level for each factor for the rest of the experiment will result in an optimum design for main effects. Note that it is permissible for intervening factors to be introduced before all the levels of a single factor are considered.

FACTORS INTRODUCED IN BLOCKS

One-at-a-time designs are of practical importance since they provide a means for minimizing the impact of a sudden unexpected termination of the experiment after any run. It may often happen, however, that the experimenter is reasonably sure that a block of runs can be completed before it is likely that the experiment must be discontinued. In such cases one might inquire how much advantage can be taken of the larger block size to improve the efficiency of the design. In answering this question attention will be confined to two-level factors.

Previous work on contractible designs has been done under the assumption that a complete block could be completed [3]. In that work a new factor is introduced in a block of runs of sufficient size that all interactions with old factors can be estimated. A number of series of such designs, both saturated and unsaturated, have been tabulated. Of necessity, each block must be of larger size than the previous. In the present paper we limit our attention to fixed block sizes.

Consider first the case in which each factor is returned to its low level after the block in which it is introduced has been completed. The matrix R for p blocks has the following form:

$$R = \begin{bmatrix} 1 & 0' & 0' & . & . & . & 0' \\ r_1 & R_{11} & 0 & & & & 0 \\ r_2 & 0 & R_{22} & & & & 0 \\ \cdot & & & \cdot & & & \cdot \\ \cdot & & & & \cdot & & \cdot \\ \cdot & & & & & \cdot & \\ r_p & 0 & 0 & . & . & . & R_{pp} \end{bmatrix}$$

The inverse, call it S, is of the same form. We have immediately $S_{ii} = R_{ii}^{-1}$ and $s_i = -S_{ii}r_i$. Note that the elements in the <u>i</u>th block of the inverse, hence the variances of the estimates, depend only on the <u>i</u>th block of the R matrix. Therefore, the problem of minimizing the variances using blocks of size k is equivalent to minimizing variances in complete designs of size k+1 . It was shown by Plackett and Burman [5] that a lower bound for the variances is $\sigma^2/(k+1)$, and that this bound is attainable if k+1 is a multiple of 4 (the case k=2 is discussed separately in a subsequent section).

By analogy with previous results (when k=1), one would expect that $\sigma^2/(k+1)$ should indeed be a lower bound for variances using blocks of size k. Similarly, by analogy with previous results, one would expect that for k+1 a multiple of 4, the lower bound should be attained if factors are held constant after the block in which they are first introduced. At present these statements are only conjectures. The next section illustrates why it may be much more difficult to complete the proofs than in the case $k=1$.

Plackett-Burman Blocks

We will be most concerned with blocks of size 3. The Plackett-Burman design for three factors in four runs is as follows:

$$X = \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \end{bmatrix} .$$

If the submatrix consisting of the last three rows and columns is used as a block (which we shall call a Plackett-Burman block of size 3), the R matrix takes the following form:

$$\begin{bmatrix} 1 & O' & O' & . & . & . & O' \\ r_1 & K & O & & & & O \\ r_2 & R_{21} & K & & & & O \\ . & & & . & & & . \\ . & & & & . & & . \\ . & & & & & . & . \\ r_p & R_{p1} & R_{p2} & . & . & & K \end{bmatrix} ,$$

where K is the matrix

$$K = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} .$$

The matrix $R^{-1} = S$ may be partitioned in the same way:

$$R^{-1} = S = \begin{bmatrix} 1 & 0' & 0' & . & . & . & 0' \\ s_1 & K^{-1} & 0 & & & & 0 \\ s_2 & S_{21} & K^{-1} & & & & 0 \\ . & & & . & & & . \\ . & & & & . & & . \\ . & & & & & . & . \\ s_p & S_{p1} & S_{p2} & . & . & . & K^{-1} \end{bmatrix} .$$

The matrix K^{-1} is

$$K^{-1} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix} ,$$

and $s_1 = -K^{-1}r_1 = -(\frac{1}{2},\frac{1}{2},\frac{1}{2})'$. If $R_{ij} = 0$ for $i > j$, then $s_i = s_1$ and the variances of the estimates of main effects are all $4(\frac{1}{2})^2\sigma^2/4 = \sigma^2/4$. Now suppose $R_{ij} = J$ for $i > j$, where J is a 3×3 matrix all of whose elements are unity. We have $S_{21} = -K^{-1}JK^{-1} = -J4$, $s_2 = -K^{-1}r_2 - K^{-1}Js_1 = r_1/4$, and in general the elements of the rows in the successive blocks can be multiples of successively higher powers of $\frac{1}{2}$. Note, however, that the variances of estimated main effects from the second block are $[3(\frac{1}{2})^2 + 4(\frac{1}{4})^2]\sigma^2/4 = \sigma^2/4$. Similarly, the variances remain at $\sigma^2/4$ for the main effects of factors in later blocks, even though the number of nonzero entries increases with each successive block. For this reason, the simple proof of Theorem 1 will not generalize directly and thus a proof that $\sigma^2/4$ is in fact the minimum variance will involve treating a number of special cases.

The picture for blocks of larger size is quite similar. For $k=7$ each diagonal block of the R matrix has the form

$$K_7 = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 \end{bmatrix} .$$

The elements of the inverse of this matrix are $\pm\frac{1}{4}$, and $s_1 = -r_1/4$. In general the elements of S_{21} are multiples of $1/16$, the elements of S_{31} are multiples of $1/64$, etc. The variances appear to have the minimum value of $1/8$ whenever factors are all held constant after the block in which they are introduced.

Blocks of Size Two

Unfortunately, nothing is gained by introducing factors two at a time over introducing them one at a time. This can be demonstrated considering the class of all non-singular 2×2 matrices whose elements are 0 and 1. Apart from permutations of rows and columns, this class consists of only two elements:

$$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} .$$

Since these matrices are themselves lower triangular, and R matrix employing blocks of size two is of exactly the same form as the R matrix for blocks of size one. Therefore, the same variance bound applies to blocks of size two as to blocks of size one.

Blocks of Size Four

It can be shown by an enumeration of possible designs that, for studying 4 two-level factors in 5 runs, the design whose R matrix is

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \end{bmatrix}$$

simultaneously minimizes the variances of the estimates. Therefore, designs using as blocks the matrix

$$K_4 = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}$$

would appear to be of primary interest. The variances of estimates of factors in the first block, obtained from

$$K_4^{-1} = \begin{bmatrix} 1/3 & 1/3 & 1/3 & -2/3 \\ 1/3 & 1/3 & -2/3 & 1/3 \\ 1/3 & -2/3 & 1/3 & 1/3 \\ -2/3 & 1/3 & 1/3 & 1/3 \end{bmatrix}$$

and $s_1 = -r_1/3$, are $(1/4 \times 8/9)\sigma^2 = 2\sigma^2/9$, which is better than can be achieved with blocks of size 3. Note that $2\sigma^2/9$ is larger than the theoretical lower bound of $\sigma^2/(k+1) = \sigma^2/5$; that bound is not attainable for 4 factor five-run designs.

By analogy with previous results, one would expect that as long as factors are held fixed after the block in which they are introduced, the variances of effects of factors in successive blocks would continue to have the same variance. Such is certainly the case if all factors are returned to their low level. Surprisingly, if some or all factors are held at their high level, variances actually decrease in subsequent blocks. In the next paragraph variances are derived as a function of block number when all factors are held at their high level.

As previously we will partition R and $S = R^{-1}$ in the form:

$$R = \begin{bmatrix} 1 & 0' & 0' & \cdots & 0' \\ r_1 & R_{11} & 0 & & 0 \\ r_2 & R_{21} & R_{22} & & 0 \\ \cdot & & & \cdot & \cdot \\ \cdot & & & \cdot & \cdot \\ \cdot & & & \cdot & \cdot \\ r_p & R_{p1} & R_{p2} & \cdots & R_{pp} \end{bmatrix}$$

$$S = \begin{bmatrix} 1 & 0' & 0' & \cdots & 0' \\ s_1 & S_{11} & 0 & & 0 \\ s_2 & S_{21} & S_{22} & & 0 \\ \cdot & & & \cdot & \cdot \\ \cdot & & & \cdot & \cdot \\ \cdot & & & \cdot & \cdot \\ s_p & S_{p1} & S_{p2} & \cdots & S_{pp} \end{bmatrix}$$

where the vectors $r_i = (1,1,1,1)'$ as usual. We are examining the case in which $R_{ii} = K_4$ and $R_{ij} = J_4$, for $i > j$, where J is the 4×4 matrix all of whose elements are unity (the subscripts 4 will be dropped). It is obvious that S_{ii} is equal to K^{-1}. It will now be shown that

$s_i = (-1/3)^i r_1$, and

$S_{ij} = 1/3(-1/3)^{i-j}J$, for $i > j$.

Formally multiplying R by S, we obtain the equations

$$r_i + \sum_{k=1}^{i} R_{ik} s_k = 0, \qquad 1 \le i \le p$$

$$\sum_{k=i}^{j} R_{ik} S_{kj} = \delta_{ij} I \; ; \qquad 1 \le i \le j \le p \; ,$$

where δ_{ij} is the Kronecker δ. Substituting the values of R_{ik} and a_k into the left side of the first equation, we obtain

$$r_i + \sum_{k=1}^{i-1} (-1/3)^k J r_1 + (-1/3)^i K r_1 .$$

Since $Jr_1 = 4r_1$ and $Kr_1 = 3r_1$, we have

$$[1 + 4 \sum_{k=1}^{i-1} (-1/3)^k + 3(-1/3)^i] r_1$$

$$= \{1 + (-1)[1-(-1/3)^{i-1}] + 3(-1/3)^i\} r_1 = 0.$$

The second of the above equations may be verified by a similar substitution for R_{ik} and S_{kj}. The variance of a main effect of a factor in the ith block is $\sigma^2/4$ times the sum of squares of the elements in the rows of $s_i, S_{i1}, S_{i2}, \ldots, S_{ii}$. This sum of squares is $(1/9)^i + \sum_{j=1}^{i-1} 4(1/9)^{i-j+1} + 7/9$, which equals $[15 + (1/9)^{i-1}]/18$. The variances, as a function of i, are as follows:

i	1	2	3	∞
variance	$.2222\sigma^2$	$.2098\sigma^2$	$.2085\sigma^2$	$.2083\sigma^2$

Note that the asymptotic variance is still larger than the conjectured lower bound of $\sigma^2/5$.

TREATING INTERACTIONS IN DESIGN FOR TWO-LEVEL FACTORS

Interactions between any 2 two-level factors may be included in the model by inclusion of a single additional run. In this section it is shown that the variance of each interaction estimate is $\frac{1}{4}\sigma^2$ and that the variance of each main effect which is included in an interaction is reduced to $\frac{1}{4}\sigma^2$.

The reduced coefficient matrix R for designs containing interactions will be constructed in a lower triangular form so as to take advantage of previous results in this paper. The portion of the R matrix relevant to two factors has one of the two forms

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} .$$

In order to estimate the interaction between the two factors it is necessary to introduce the fourth possible combination of levels for the two factors. The interaction will be assigned the value 1 in the R matrix when the fourth combination appears and 0 for the other three combinations. Thus, the portion of R corresponding to two factors and their interaction has one of the two forms

$$R^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \quad \text{or} \quad R^{(2)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \end{bmatrix} .$$

These are related to the traditional coefficient matrices through trianguler transformation matrices as follows:

$$X^{(1)} = \begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & -1 & -1 & 1 \\ 0 & 2 & 0 & -2 \\ 0 & 0 & 2 & -2 \\ 0 & 0 & 0 & 4 \end{bmatrix} = R^{(1)}T^{(1)}$$

$$X^{(2)} = \begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & -1 & -1 & 1 \\ 0 & 2 & 0 & -2 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & -4 \end{bmatrix} = R^{(2)}T^{(2)} .$$

The inverses of these transformation matrices are respectively

$$(T^{(1)})^{-1} = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{2} & 0 & \frac{1}{4} \\ 0 & 0 & \frac{1}{2} & \frac{1}{4} \\ 0 & 0 & 0 & \frac{1}{4} \end{bmatrix} \quad \text{and} \quad (T^{(2)})^{-1} = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{2} & 0 & -\frac{1}{4} \\ 0 & 0 & \frac{1}{2} & \frac{1}{4} \\ 0 & 0 & 0 & -\frac{1}{4} \end{bmatrix} .$$

The transformation matrices for general one-at-a-time designs containing n factors, m interactions, and $n + m + 1$ runs are of the general form

$t_{11} = 1$

$t_{1j} = -1 \quad (j = 2,\ldots,n + 1)$

$t_{1j} = 1 \quad (j = n + 2,\ldots,n + m + 1)$

$t_{jj} = 2 \quad (j = 2,\ldots,n + 1)$

$t_{jj} = \pm 4 \quad (j = n + 2,\ldots,n + m + 1)$

$t_{ij} = \pm 2 \quad$ ($j = n + 2,\ldots,n + m + 1$ and the ($\underline{i-1}$)st factor is involved in the interaction corresponding to the $\underline{j}$th column)

$t_{ij} = 0 \quad$ (otherwise).

The elements of $V = T^{-1}$ are of the general form

$v_{11} = 1$

$v_{1j} = \frac{1}{2} \quad (j = 2,\ldots,n + 1)$

$v_{1j} = \frac{1}{4} \quad (j = n + 2,\ldots,n + m + 1)$

$v_{jj} = \frac{1}{2} \quad (j = 2,\ldots,n + 1)$

$v_{jj} = \pm\frac{1}{4} \quad (j = n + 2,\ldots,n + m + 1)$

$v_{ij} = \pm\frac{1}{4} \quad$ ($j = n + 2,\ldots,n + m + 1$ and the ($\underline{i-1}$)st factor is involved in the interaction corresponding to the $\underline{j}$th column)

$v_{ij} = 0$ (otherwise).

Since the variance of an estimated parameter is σ^2 times the sum of squares of the elements of a row of $X^{-1} = T^{-1}R^{-1}$, and since T^{-1} contains elements as small as $\frac{1}{4}$, an argument like that used to prove Theorem 1 can be used to show that a variance could have a value as low as $\frac{1}{4}\sigma^2$. For those factors which are involved in no interaction, however, the corresponding row of T^{-1} contains only the values $\frac{1}{2}$ and 0, so that the variance bound is the same as before.

It remains to determine whether or not designs exist for which the bound of $\frac{1}{4}\sigma^2$ is attained. Once again the answer is in the affirmative, and those designs for which factors are returned to their low levels after their initial introduction except for runs in which they are involved in the interaction have the optimum property. As an example, consider a design for estimating the effects of four factors and the interactions between the first and third and third and fourth. The R matrix for such a design is as follows:

$$R = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 \end{bmatrix} .$$

The matrix is easily inverted to obtain

$$S = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 & -1 & 0 & 1 \end{bmatrix} ,$$

which when multiplied by T^{-1} yields

$$X^{-1} = \begin{bmatrix} -\frac{1}{2} & \frac{1}{4} & \frac{1}{2} & 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ -\frac{1}{4} & \frac{1}{4} & 0 & -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 & \frac{1}{4} & \frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & 0 & 0 & -\frac{1}{4} & \frac{1}{4} & 0 & \frac{1}{4} \\ \frac{1}{4} & -\frac{1}{4} & 0 & -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ -\frac{1}{4} & 0 & 0 & \frac{1}{4} & -\frac{1}{4} & 0 & \frac{1}{4} \end{bmatrix} .$$

The variance of the interaction estimates and of the main-effect estimates are all $\frac{1}{4}\sigma^2$ except for the factor which is involved in no interaction, for which the variance is $\frac{1}{2}\sigma^2$.

A WORD OF WARNING

It has been the purpose of this paper to present general results on saturated sequential designs such as one-at-a-time designs. It will be appropriate, however, to make a few observations on their limitations.

By their very nature, the designs discussed have all their degrees of freedom used in estimating effect parameters, so that no internal error estimate is available. Sometimes this may be no particular disadvantage. Either a good error estimate is available from prior experience, or it is not required of the experiment to test the significance the parameter estimates relative to the error. Alternatively, the half-normal plotting procedure, due to Daniel [6], may be used if only a few of the factors are expected to have real effects.

Since the runs are conducted in a sequential fashion, with the possibility of altering the experiment between runs, there is no opportunity to obtain a complete randomization of the order of the runs. Rather than attempting to obtain a "partial randomization" by, for example, randomizing the order of introduction of some of the factors, the experimenter should introduce the factors in the order of their potential importance. It is obvious that in the absence of a complete randomization, there is no basis for the validity of tests for significance of the estimated effects. Thus, these designs do not provide a statistical proof of the reality of effects. They will, however, give an indication of what are apt to be the most important factors. A standard design, fully randomized, can be run subsequently in order to provide valid significance tests.

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13. ABSTRACT

The report consists of three distinct but related papers. The first is concerned with methods for constructing designs to meet realistic requirements on the number of runs and with criteria for selecting a design from a number of alternatives. Examples of various construction techniques are illustrated and designs are given which were constructed for actual experiments. Two specific numerical criteria are developed, and a convenient computer routine for evaluating them is described.

The second paper discusses designs of even resolution. It is shown that the smallest resolution 4 designs for n factors at two levels must contain at least 2n runs, and that "foldover" designs are available with 2n runs. It is conjectured that the only minimal resolution 4 designs are foldover designs. The case of resolution 6 designs is also discussed.

The third paper gives the variance bounds for estimates of main effects using one-at-a-time designs, and characterizes those designs which achieve the lower bounds. Situations in which runs are conducted a block at a time (rather than singly) are treated and it is shown that inclusion of interaction terms in the model improves the main-effect estimates of factors involved in the interactions.

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