VICTORIA UNIVERSITY
OF TECHNOLOGY

DEPARTMENT OF
MATHEMATICS, COMPUTING
AND OPERATIONS RESEARCH

THE USE OF A CLASS OF FOLDOVER DESIGN AS SEARCH DESIGNS

Neil T. Diamond

(1 EQRM 1)

September 1990

TECHNICAL REPORT

DEPT OF MCOR
FOOTSCRAY INSTITUTE OF TECHNOLOGY
VICTORIA UNIVERSITY OF TECHNOLOGY
BALLARAT ROAD (P O BOX 64), FOOTSCRAY
VICTORIA, AUSTRALIA 3011
TELEPHONE (03) 688-4249/4225
FACSIMILE (03) 687-7632

THE USE OF A CLASS OF FOLDOVER DESIGN AS SEARCH DESIGNS

Neil T. Diamond

(1 EQRM 1)

September 1990

Efficiency, Quality and Reliability
Management Centre

This paper has been accepted for publication in
The Australian Journal of Statistics

THE USE OF A CLASS OF FOLDOVER DESIGNS AS SEARCH DESIGNS

NEIL T. DIAMOND

It is shown that a class of two-level nonorthogonal resolution IV designs with n factors are strongly resolvable search designs when k, the maximum number of two-factor interactions thought possible, equals one; weakly resolvable when $k = 2$ except when the number of factors is 6; and may not be weakly resolvable when $k \geq 3$.

Key words: Fractional factorial designs; nonorthogonal designs; resolution IV designs; search designs.

1. Introduction.

Resolution IV designs allow the estimation of all main effects clear of the bias due to non-zero two-factor interactions. The most common designs used in practice and discussed in the literature are orthogonal and for these designs the two-factor interactions are aliased with each other.

Margolin (1969) has discussed the use of nonorthogonal resolution IV designs involving n two-level factors in 2n runs which for most values of n would involve fewer runs with a small sacrifice in the efficiency of the estimation of the main effects. However, as is shown below, these non-orthogonal designs may allow the search and estimation of a small number of non-zero two-factor interactions when considered as search designs.

2. Search Designs.

Srivastava (1975) pointed out that the factorial effects in an experiment can be divided into three categories:

(i) effects that we are sure are negligible,
(ii) effects that we want to estimate, and
(iii) the remaining effects, most of which are negligible, but a few of which may be non-negligible.

Designs which provide estimates of all effects of type (ii) and enable a search for the non-negligible effects from type (iii), on the assumption that there is no error, are called strongly resolvable search designs. If the search can only be carried out for some values of the non-zero interactions then the design is called weakly resolvable.

Srivastava showed that a necessary and sufficient condition for a 2^n factorial design to be strongly resolvable when the maximum number of non-negligible effects is k, is that every submatrix of the design matrix consisting of all the columns corresponding to the effects of type (ii) and 2k of the columns corresponding to the effects of type (iii) is of full rank.

3. Modified One Factor at a Time Foldover Designs.

The class of resolution IV designs considered here is generated by using the foldover theorem established by Box and Wilson (1951,p.35) who showed that folding over any resolution III design involving (n-1) factors results in a resolution IV design involving n factors. Take, for example, the case when n = 5. The classical one factor at a time design involving 4 factors, A, B, C and D, is a resolution III design and consists of the runs {(1), a, b, c, d}. Replacing the first run of this design, where all the factors are at their low level, by the run where all the factors are at their high level, in this case abcd, the design {abcd, a, b, c, d} is obtained. John (1971, p172) has shown that this construction leads to a design also of resolution III which is always more efficient than the one factor at a time design for all values of n. We will call such a design a modified one factor at a time design.

The modified one factor at a time foldover design consists of the modified one factor at a time design and the foldover of that design, with an additional factor incorporated set at its low level in the modified one factor at a time design and at its high level in the foldover. With n = 5 the design is given by the runs {abcd, a, b, c, d, e, bcde, acde, abde, abce}. In fact, for all values of n, the designs are given by all one-letter runs and all (n-1)-letter runs.

It is easy to show that the variances of the main effect estimates in these designs are given by $(n^2 - 5n + 8)/[2(n - 2)^2]\sigma^2$. We can compare these values to those given in Table 2 of Margolin's paper where the main effect variances of the most efficient non-orthogonal resolution IV designs given in the literature are tabulated. It needs to be stressed, however, that since Margolin defines an effect of a factor A as half the difference between the average response at the high level of A and the average response at the low level of A, which is one half the usually defined A effect, Margolin's variances need to be multiplied by four for a proper comparison. Making this comparison it can be seen that the modified one factor at a time foldover designs appear to be quite efficient when the number of factors is between 3 and 7. For $n = 3, 5$ and 7 the effect variances match the values presented by Margolin while for $n = 6$ the effect variance for the design is $0.4375\sigma^2$ which is only slightly higher than the tabulated value of $0.4\sigma^2$. The case when $n = 4$ is in fact the orthogonal 2^{4-1} design with defining contrast $I = -ABCD$ which gives main effect estimates with 100% efficiency. Since many industrial experiments do involve between 3 and 7 factors an examination of these designs appears to be worthwhile.

However as the number of factors increases it should be noted that the designs generated by folding over the resolution III designs given by Yang (1966,1968) become increasingly more efficient than the designs considered in this paper. The Yang foldovers have effect variances of $\sigma^2 / (2n - 2)$ for $n = 2 \pmod 4$. Research on the use of the Yang foldovers as search designs is currently in progress.

4. Searching For Non-negligible Two-factor Interactions.

For the modified one factor at a time foldover designs, with the assumption that all three-factor and higher interactions are negligible, the design matrix is of the form

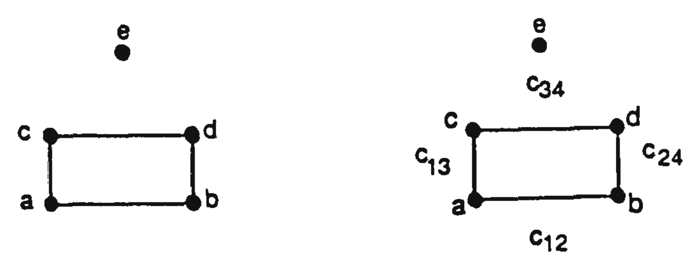
$$X = \begin{bmatrix} 1 & U & V \\ 1 & -U & V \end{bmatrix}$$

where $1\ (n \times 1) = (1, 1, \ldots\ldots 1)'$, $U\ (n \times n)$ has 1's on the diagonal and -1's elsewhere and V denotes the matrix of the $n(n - 1)/2$ two-factor interaction effects where the column corresponding to the interaction between the ith and jth factors has -1's in the ith and jth rows and +1's elsewhere.

We want to estimate the mean and the main effects and search over and estimate the non-zero two factor interactions. To show that the design is of resolving power k the rank of all matrices Y, consisting of the first (n + 1) columns of X and 2k of the last n(n - 1)/2 columns of X, must be (n+1+2k). However, Webb (1968) has shown that the columns corresponding to the main effects in any resolution IV design are linearly independent of one another, and are orthogonal to, and therefore linearly independent of, the columns corresponding to the mean and the two-factor interactions. We can also centre the columns corresponding to the two-factor interactions to make them orthogonal to the mean and hence we only have to show that every 2k columns of the n x [n(n-1)/2] matrix W = V - [(n-4)/n]J have full rank, where J is the n x [n(n-1)/2] matrix whose every element is 1.The column of W corresponding to the interaction between the ith and jth factors, β_{ij}, takes the values (4-2n)/n in the ith and jth rows and 4/n elsewhere.

It turns out that in order to determine whether a set of the β_{ij}'s is linearly independent or not it is very useful to form the columns $\alpha_{ij} = (2/n) - 0.5\beta_{ij}$ which take the values 1 in the ith and jth rows and 0 elsewhere. The matrix of the α_{ij} corresponding to a set of 2k two-factor interactions is in fact an incidence matrix of a graph with n vertices and 2k edges. Each vertex of the graph corresponds to one of the runs a, b, c, ..., and an edge between two vertices is present if the interaction involving the same letters as the vertices is in the set. In addition a linear combination of the α_{ij} say $\Sigma\Sigma\, c_{ij}\, \alpha_{ij}$ can be represented as a weighted graph or network, where the weight c_{ij} is assigned to the edge corresponding to α_{ij}. Figure 1 shows for n = 5 the graph and network corresponding to the set of two factor interactions {AB, AC, BD, CD} and the linear combination $(c_{12}\alpha_{12} + c_{13}\alpha_{13} + c_{24}\alpha_{24} + c_{34}\alpha_{34})$ respectively.

Figure 1: Graph corresponding to {AB, AC, BD, CD} and Network corresponding to $c_{12}\,\alpha_{12} + c_{13}\,\alpha_{13} + c_{24}\,\alpha_{24} + c_{34}\,\alpha_{34}$ for n = 5.



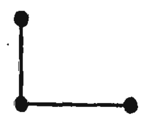
Since the α_{ij} take the values 1 in the ith and jth rows and 0 elsewhere, the result of the above linear combination will be $(c_{12}+c_{13}, c_{12}+c_{24}, c_{13}+c_{34}, c_{24}+c_{34}, 0)'$, that is each element of the vector can be obtained by simply summing the weights of the edges incident with the corresponding vertex. This method of representing a linear combination gives a very easy way of checking whether the columns associated with a set of interactions are linearly dependent since, as is shown below, a linear combination of the β_{ij}'s is zero if and only if a set of weights can be found so that the sums of the weights at each of the vertices are the same, that is $\Sigma\Sigma\, c_{ij}\, \alpha_{ij} = (x, x,..., x)'$ for some real x. To prove the if part assume $\Sigma\Sigma\, c_{ij}\, \alpha_{ij} = (x, x, ..., x)'$. Then $\Sigma\Sigma\, c_{ij}\, (2/n - 0.5\, \beta_{ij}) = (x, x, ..., x)'$ and hence $\Sigma\Sigma\, c_{ij}\, \beta_{ij} = (4\Sigma\Sigma\, c_{ij}/n - 2x, ..., 4\Sigma\Sigma\, c_{ij}/n - 2x)'$. But $\Sigma\Sigma\, c_{ij} = nx/2$ since the weights incident to every vertex add to x, there are n vertices and every edge is incident to two vertices. Hence $\Sigma\Sigma\, c_{ij}\beta_{ij} = (0, 0,.., 0)'$. To prove the only if part assume $\Sigma\Sigma\, c_{ij}\beta_{ij} = (0, 0, ..., 0)'$. Hence $\Sigma\Sigma\, c_{ij}\, (4/n - 2\alpha_{ij}) = (0, 0, ...0)'$ and therefore $\Sigma\Sigma\, \alpha_{ij}\, c_{ij} = (x, ..., x)'$ with $x = 2\, \Sigma\Sigma\, c_{ij}/n$. This is a very useful result that allows the determination of the linear dependence or independence of a set of interaction columns via the examination of the associated graph.

4.1 k = 1.

To show that the designs are strongly resolvable when k = 1 all the possible graphs with n vertices and 2 edges need only be considered. Since these designs are symmetric in each of the factors, in the sense that interchange of factor labels does not alter the design, it is only necessary to consider unlabelled graphs. In general, the number of graphs with n vertices and q edges for $n \geq 2q$ equals the number of graphs with 2q vertices and q edges because any additional vertices over 2q only increases the number of isolated vertices.

Since the number of graphs with 4 vertices and 2 edges is 2, see for example Harary (1972, p.214), there are only two cases to consider which are given on p.215 of Harary and summarised in Table 1.

Table 1: All graphs with n vertices and 2 edges

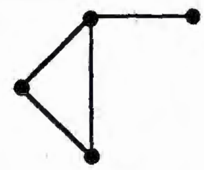
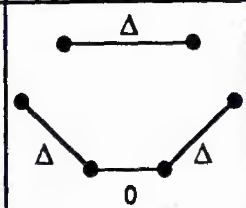
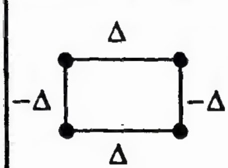
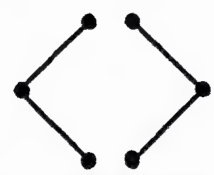
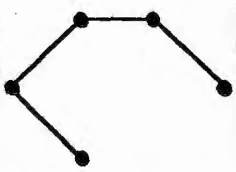
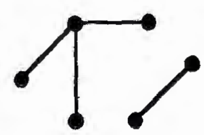
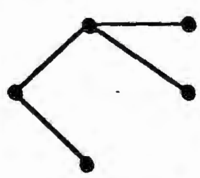
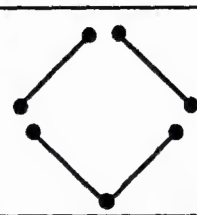
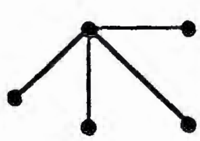
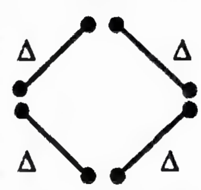
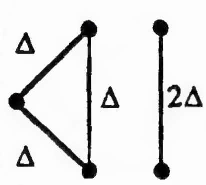
Case	Graph	Number of isolated Vertices
1		(n - 3)
2		(n-4)

It is clearly not possible to assign non-zero weights to the edges so that the sums of the weights at each of the vertices are the same except when n = 4. Searching for at most one non-zero interaction is thus possible apart from the case when n = 4 corresponding to the orthogonal 2^{4-1} design.

4.2 k = 2.

All the possible unlabelled graphs with n vertices and 4 edges need to be considered where n ≥ 5, since there are at most 3 edges when n = 3 and the case n = 4 corresponds to the standard orthogonal design. Again from p. 215 of Harary the number of cases to consider is 11. The first 9 cases are given on p. 218 of Harary and these together with the last two cases, found using trial and error, are summarised in Table 2 with weights assigned to the edges where the set of interactions are dependent:

Table 2: All graphs with n vertices and 4 edges.

<table>
<tr><th>Case</th><th>Graph</th><th>Number of Isolated Vertices</th><th>Case</th><th>Graph</th><th>Number of Isolated Vertices</th></tr>
<tr><td>1</td><td></td><td>(n - 4)</td><td>7</td><td></td><td>(n - 6)</td></tr>
<tr><td>2</td><td></td><td>(n - 4)</td><td>8</td><td></td><td>(n - 6)</td></tr>
<tr><td>3</td><td></td><td>(n - 5)</td><td>9</td><td></td><td>(n - 6)</td></tr>
<tr><td>4</td><td></td><td>(n - 5)</td><td>10</td><td></td><td>(n - 7)</td></tr>
<tr><td>5</td><td></td><td>(n - 5)</td><td>11</td><td></td><td>(n - 8)</td></tr>
<tr><td>6</td><td></td><td>(n - 5)</td><td></td><td></td><td></td></tr>
</table>

Case 2 is dependent for all values of n. Cases 6, 7 and 11 are dependent only for n = 5, 6 and 8 respectively. All the other cases are independent. The dependent cases can be used to show when searching for at most two non-zero interactions is not possible.

For example from case 2 with n = 5 we can see that $(\Delta\alpha_{12} - \Delta\alpha_{13} - \Delta\alpha_{24} + \Delta\alpha_{34}) = (0, 0, ..., 0)'$ and also $(\Delta\alpha_{12} - \Delta\alpha_{13} - \Delta\alpha_{25} + \Delta\alpha_{35}) = (0, 0, ..., 0)'$, for arbitrary Δ, and therefore $\Delta\beta_{12} - \Delta\beta_{13} - \Delta\beta_{24} + \Delta\beta_{34} = \Delta\beta_{12} - \Delta\beta_{13} - \Delta\beta_{25} + \Delta\beta_{35} = (0, 0, ..., 0)'$. If we consider the case where the interaction effects are AB = Δ and AC = - Δ, all other interactions being zero, then the component of the observation vector orthogonal to the mean and main effects is given by $\Delta\beta_{12} - \Delta\beta_{13} = \Delta\beta_{24} - \Delta\beta_{34} = \Delta\beta_{25} - \Delta\beta_{35}$ and therefore the true Model {AB, AC}, with AB = Δ and AC = -Δ, cannot be distinguished from the false models {BD, CD}, with BD = Δ and CD = - Δ, and {BE, CE}, with BE = Δ and CE = - Δ, on the basis of the data.

As another example, from case 6 with n = 5, we can see that $(\Delta\alpha_{12} + \Delta\alpha_{13} + \Delta\alpha_{23} + 2\Delta\alpha_{45}) = (2\Delta, 2\Delta, ..., 2\Delta)'$ and therefore $(\Delta\beta_{12} + \Delta\beta_{13} + \Delta\beta_{23} + 2\Delta\beta_{45}) = (0, 0, ..., 0)'$. If we consider the case where the interaction effects are AB = Δ and AC = Δ, all other interactions being zero, then the component of the observation vector orthogonal to the mean and main effects is given by $\Delta\beta_{12} + \Delta\beta_{13} = - \Delta\beta_{23} - 2\Delta\beta_{45}$ and therefore the true model {AB, AC} , with AB = Δ and AC = Δ, cannot be distinguished from the false model {BC, DE}, with BC = - Δ and DE = - 2Δ, on the basis of the data.

A complete examination of Table 2 shows that searching is not possible only for the following true models:

1. The true model consists of two interactions with one letter in common where:
   (a) the interaction effects are equal in magnitude but opposite in sign,
   or (b) the interaction effects are equal and $n = 5$.

or

2. The true model consists of two interactions with no letters in common where:
   (a) the interaction effects are equal,
   or (b) one of the interaction effects is twice the other interaction effect and $n = 5$.

or

3. The true model consists of only one interaction and $n = 6$:

In the latter case, which follows from case 7 of Table 2, the design is not even weakly resolvable, since if the true model is {AB} with AB = Δ, say, then the true model cannot be separated from the model {CD, EF}, with CD = - Δ and EF = - Δ, and other models under an interchange of letters, irrespective of the value of Δ. It should be noted that case 7 is only dependent when a zero weight is assigned to the edge specified in Table 2 and this is equivalent to dropping the corresponding interaction from the Model being considered.

4.3 $k = 3$.

Examination of case 2 of Table 2 shows that for any value of n the design may not be even weakly resolvable, for if the true model consists of one interaction, say AB, with value Δ then it is not possible to separate it from the false model with {BD, AC, CD} where BD = Δ, AC = Δ and CD = - Δ.

5. Conclusion.

The results of the previous section show that if $k = 1$, then the designs considered here are perfectly satisfactory, at least in the error-free case. If $k = 2$ and $n \neq 6$ then the designs will be satisfactory unless the parameter values of the two factor interactions take on certain values, in which case an augmenting design, along the lines of those used by Daniel (1962,1976 Chapter 14) for orthogonal resolution IV designs, would need to be run. The main advantage of these designs over the usual orthogonal fractional replicates is that on many occasions no augmenting designs will be required.

If $k = 2$, $n = 6$ and, if only one interaction is non-zero, augmenting will be required irrespective of the value of the interaction effect. If two interactions are non-zero augmenting will only be required when the interactions take on certain values. The case when $k = 3$ is similar in that when only one interaction is non-zero augmenting will be required but if two or three interactions are non-zero augmenting will only be required for certain parameter values.

These results indicate that the designs considered here should not be used when $k = 2$ and $n = 6$ or when $k = 3$ since their major advantage over the orthogonal designs may be absent.

Finally, the performance of the designs when error is present and the design of augmenting trials, when required, will be reported in a subsequent paper.

Acknowledgements:

This work was completed as part fulfilment of the author's Ph.D currently in progress in the Department of Statistics at the University of Melbourne. I would like to thank my supervisor, Dr. Ken Sharpe, for his help and encouragement.

References:

Box, G.E.P. and K.B. Wilson. (1951), On the experimental attainment of optimal conditions, J. Roy. Stat. Soc., Series B, 13, 1 - 45

Daniel, C. (1962), Sequence of fractional replicates in the 2^{p-q} series, J. Am. Stat. Soc., 58, 403 - 429

Daniel, C. (1976), Applications of Statistics to Industrial Experimentation, New York : John Wiley & Sons

Harary, F. (1972), Graph Theory. Reading, Massachusetts : Addison - Wesley

John, P.W.M. (1971), Statistical Design and Analysis of Experiments, New York : MacMillan Co.

Margolin, B.H. (1969), Results on factorial designs of Resolution IV for the 2^n and $2^n 3^m$ Series, Technometrics, 11, No. 3, 431 - 444

Srivastava, J.N. (1975) Designs for searching non-negligible effects, in J.N. Srivastava, ed. A Survey of Statistical Design and Linear Models, North-Holland Publishing Company.

Webb, S. (1968), Non-orthogonal designs of even resolution, Technometrics, 10, No.2, 291-299.

Yang, C.H. (1966), Some designs for maximal (+1,-1)- determinant of order n = 2 (mod 4), Mathematics of Computation, 20, 147-148.

Yang, C.H. (1968), On designs of maximal (+1,-1)- matrices of order n = 2 (mod 4), Mathematics of Computation, 22, 174-180.