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FOLDOVER SEARCH DESIGNS

WITH ERROR AND AUGMENTING RUNS

Neil T. Diamond

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VICTORIA UNIVERSITY OF TECHNOLOGY
BALLARAT ROAD (P O BOX 64) FOOTSCRAY
VICTORIA, AUSTRALIA 3011
TELEPHONE (03) 688-4249/4492
FACSIMILE (03) 687-7632

Campuses at
Footscray, Melton,
St Albans, Werribee

FOLDOVER SEARCH DESIGNS WITH ERROR AND AUGMENTING RUNS

Neil T. Diamond*
Victoria University of Technology

Summary

The performance of a class of two-level nonorthogonal resolution IV designs with n factors when experimental error is present is investigated and the design of augmenting trials discussed and illustrated with an example. If a block effect needs to be taken into account then only two augmenting trials are required with up to five factors and three augmenting trials with up to nine factors.

Key Words: Fractional factorial designs; nonorthogonal designs; resolution IV designs.

1. Introduction

The most common resolution IV designs used in practice and discussed in the literature are orthogonal. For these designs the main effects are estimable and unbiased by two-factor interactions while the two-factor interactions are usually aliased with each other.

*Department of Computer and Mathematical Sciences, Victoria University of Technology–Footscray, PO Box 14428, Melbourne Mail Centre, Melbourne, Vic. 3000, Australia. *Acknowledgements.* The author thanks Dr Ken Sharpe for his help and encouragement with this work, which is part of the author's Ph.D. currently in progress at the Dept. Statistics, University of Melbourne.

In a previous paper, (Diamond, 1991), it was shown that the class of modified one-factor-at-a-time foldover designs, consisting of all one-letter runs and all $(n-1)$-letter runs for n two-level factors, can be considered as search designs (Srivastava, 1975). When there is no error a strongly resolvable search design of resolving power k provides, in this context, estimates of the mean and all main effects and allows the search and estimation of the real two-factor interactions, assuming the maximum number of real two-factor interactions is k; while a weakly resolvable search design only allows this for some values of the two-factor interactions. The modified one-factor-at-a-time foldover designs are strongly resolvable when $k = 1$; weakly resolvable when $k = 2$ except when the number of factors is 6; and may not be even weakly resolvable when $k \geq 3$.

In this paper the above results are extended to cover the case when experimental error is present and also to illustrate the design of augmenting trials which may be needed if the real two-factor interactions take on certain values.

2. An Example

Box, Hunter and Hunter (1978, p.377) illustrated the use of a 2^{5-1} fractional factorial design by re-analysing a 2^5 design but only using the results of the runs in the 2^{5-1} design. The five factors were **1**, feed rate; **2**, catalyst; **3**, agitation rate; **4**, temperature; and **5**, concentration; while the response was the percentage of a raw material reacted in a reactor. For convenience in this paper the five factors have been re-labelled B, D, C, A and E respectively.

Table 1 gives the results of the ten runs in the 2^5 experiment corresponding to the modified one-factor-at-a-time foldover design. Table 2 gives the mean square errors for the regression of the five main effects on the response and also for the best five models when fitting one and two interactions in addition to the main effects where, for example, $\{AD, AE\}$ corresponds to the model where the main effects A to E are fitted as well as the two-factor interactions AD and AE.

Examination of Table 2 reveals a very interesting feature. The three models $\{AD,AE\}$, $\{BD,BE\}$, and $\{CD,CE\}$ show a sizeable reduction in the mean square error over models involving only one two-factor interaction and, in addition, there appears to be a clear gap to other models involving

Run	Factor					Response
	A	B	C	D	E	(% reacted)
1	+	−	−	−	−	69
2	−	+	−	−	−	53
3	−	−	+	−	−	53
4	−	−	−	+	−	63
5	−	−	−	−	+	56
6	−	+	+	+	+	65
7	+	−	+	+	+	81
8	+	+	−	+	+	77
9	+	+	+	−	+	42
10	+	+	+	+	−	98

Table 1: Results of the 10 runs in a 2^5 experiment corresponding to the modified one-factor-at-a-time foldover design.

Number of interactions	Interactions in model	*MSE*
0	$\{\}$	152.90
1	$\{CD\}$	96.53
	$\{BE\}$	115.67
	$\{AE\}$	115.67
	$\{BD\}$	125.19
	$\{AD\}$	125.19
2	$\{CD, CE\}$	1.79
	$\{AD, AE\}$	5.50
	$\{BD, BE\}$	5.50
	$\{AE, BC\}$	52.00
	$\{AC, AE\}$	52.00

Table 2: Mean square errors for the model with main effects only, and the best five models involving the main effects and, in addition, one and two interactions respectively.

two two-factor interactions. If we assume that there are at most two non-zero two-factor interactions then it appears likely that one of these three models is the correct one. Analysis of the full 2^5, with the regression parameterization used in this paper, shows that the true model is in fact $\{AD,AE\}$ with $\widehat{AD} = 6.625$ and $\widehat{AE} = -5.5$.

The fact that these three models are the best is in line with the findings in the previous paper. There it was shown that when the true model consists of two interactions with one letter in common and the interaction effects equal in magnitude but opposite in sign, then searching for the true model in the error-free case is not possible since the component of the observation vector orthogonal to the mean and main effects lies in the subspaces corresponding to a number of different models. The example illustrates that, even when the interaction effects are only approximately equal in magnitude and opposite in sign, it will be difficult to distinguish between the models corresponding to the intersecting subspaces on the basis of the data if error is present. As shown in a later section it is possible to design augmenting trials to resolve these ambiguous results.

3. Performance of the Designs with Error

In the example a number of models had similar mean square errors. In this section an analysis of the expected value of the mean square error when fitting a false model will be undertaken and applied to the modified one-factor-at-a-time foldover design.

Consider the case where we are fitting a model M_2 when the true model is in fact M_1. In the context considered in this paper M_1 and M_2 would involve the mean, all main effects and $k_i (i = 1, 2) < (n - 1)$ two factor interactions respectively where the two factor interactions are different for M_1 and M_2.

The true and false models can be rewritten as

$$\begin{aligned} M_1 : y &= X_0\beta_0 + X_1\beta_1 + \varepsilon_1 \\ M_2 : y &= X_0\beta_0 + X_2\beta_2 + \varepsilon_2 \end{aligned}$$

where $X_0(2n \times (n+1))$ consists of the columns of the design matrix corresponding to the mean and main effects, $X_1(2n \times k_1)$ and $X_2(2n \times k_2)$ consist of the remaining columns of the design matrices respectively and $\varepsilon_1 \sim N(0, \sigma^2 I)$ since M_1 is the true model whereas $\varepsilon_2 \sim N(X_1\beta_1 - X_2\beta_2, \sigma^2 I)$. Both models can be rewritten as

$$\begin{aligned} M_1 : y_{\cdot 0} &= X_{1\cdot 0}\beta_1 + \varepsilon_1 \\ M_2 : y_{\cdot 0} &= X_{2\cdot 0}\beta_2 + \varepsilon_2 \end{aligned}$$

where $y_{\cdot 0}$, $X_{1\cdot 0}$ and $X_{2\cdot 0}$, the matrices of residuals of y,X_1 and X_2 regressed on X_0 respectively are given by

$$\begin{aligned} y_{\cdot 0} &= (I - X_0(X_0'X_0)^{-1}X_0')y \\ X_{1\cdot 0} &= (I - X_0(X_0'X_0)^{-1}X_0')X_1 \\ X_{2\cdot 0} &= (I - X_0(X_0'X_0)^{-1}X_0')X_2. \end{aligned}$$

When model M_2 is fitted then $y_{\cdot 0}$ is projected onto the manifold generated by the columns of $X_{2\cdot 0}$. Then the estimated error vector $\hat{\varepsilon}_2$ is given by

$$\hat{\varepsilon}_2 = (I - P)(X_{1\cdot 0}\beta_1 + \varepsilon_1)$$

where the projection operator is

$$P = X_{2\cdot 0}(X_{2\cdot 0}'X_{2\cdot 0})^{-1}X_{2\cdot 0}'.$$

The residual sum of squares is then given by

$$\begin{aligned} RSS &= \hat{\varepsilon}_2'\hat{\varepsilon}_2 \\ &= (\beta_1'X_{1\cdot 0}' + \varepsilon_1')(I - P)(X_{1\cdot 0}\beta_1 + \varepsilon_1) \end{aligned}$$

since $(I - P)$ is idempotent. Hence

$$\begin{aligned} E(RSS) &= E(\beta_1'X_{1\cdot 0}' + \varepsilon_1')(I - P)E(X_{1\cdot 0}\beta_1 + \varepsilon_1) + \text{trace}(\sigma^2(I - P)I) \\ &= \beta_1'X_{1\cdot 0}'(I - X_{2\cdot 0}(X_{2\cdot 0}'X_{2\cdot 0})^{-1}X_{2\cdot 0}')X_{1\cdot 0}\beta_1 + (n - k_2 - 1)\sigma^2. \end{aligned}$$

In table 3 the expected values of the mean square errors have been calculated using the above formula for the cases where if there were no error then more than one model could fit the data exactly.

n	True Model	False Models	$E(MSE)$ for False Models
≥ 5	$\{AB, AC\}$	$\{BD, CD\}, \{BE, CE\}, \ldots$	$\sigma^2 + \frac{32(n-4)(AB+AC)^2}{(3n-8)(n-3)}$
≥ 5	$\{AB, CD\}$	$\{AC, BD\}, \{AD, BC\}$	$\sigma^2 + \frac{8(AB-CD)^2}{(n-3)}$
5	$\{AB, AC\}$	$\{BC, DE\}$	$\sigma^2 + 2(AB - AC)^2$
5	$\{AB, CD\}$	$\{AE, BE\}, \{CE, DE\}$	$\sigma^2 + \frac{8}{7}(2AB - CD)^2$
6	$\{AB\}$	$\{CD, EF\}$	σ^2
6	$\{AB, CD\}$	$\{EF\}$	$\sigma^2 + \frac{8}{3}(AB - CD)^2$
8	$\{AB, CD\}$	$\{EF, GH\}$	$\sigma^2 + \frac{8}{5}(AB - CD)^2$

Table 3: $E(MSE)$ for various false models for the modified one-factor-at-a-time foldover design involving n factors.

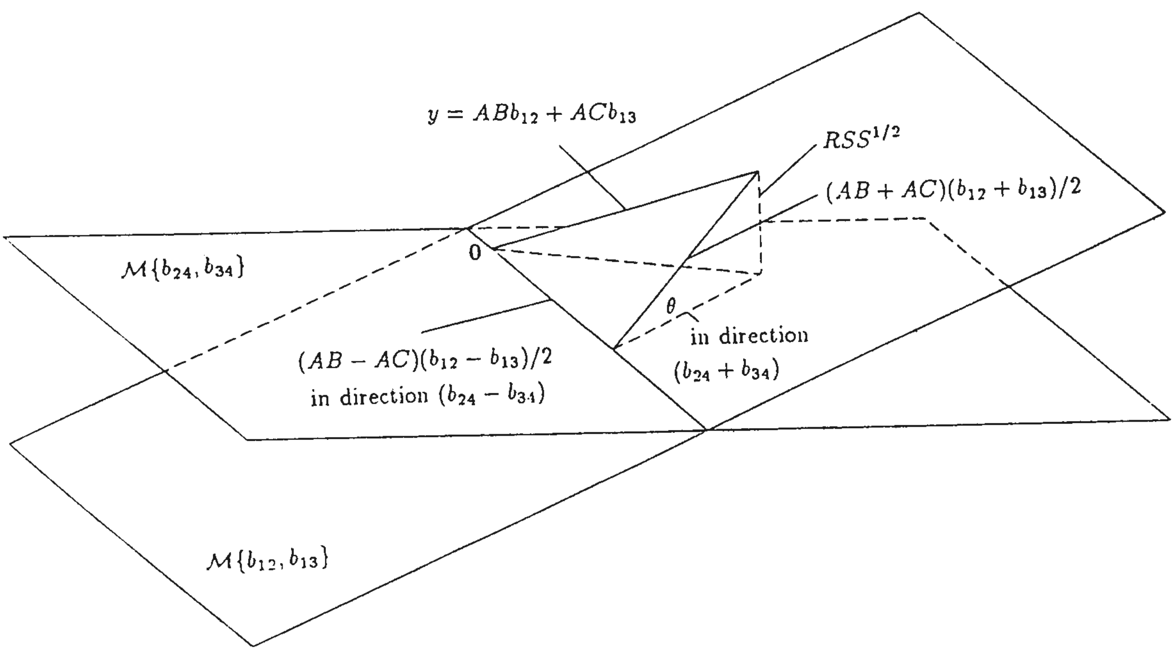

Figure 1: Geometric interpretation of the estimation of the two-factor interactions BD and CD when the real two-factor interactions are in fact AB and AC, following a modified one-factor-at-a-time foldover design.

Table 3 shows, for example, that if the true model is $\{AB, AC\}$ and if $AB = -AC$ then the expected value of the mean square errors will be σ^2 for $(n-2)$ models. A geometric interpretation of this result and an alternative derivation of $E(RSS)$ is given below and represented in Figure 1.

The manifold orthogonal to the mean and main effects corresponding to the true model $\{AB, AC\}$ is spanned by the vectors b_{12} and b_{13} and is denoted by $\mathcal{M}\{b_{12}, b_{13}\}$, while the manifold orthogonal to the mean and main effects corresonding to the false model $\{BD, CD\}$ say is spanned by the vectors b_{24} and b_{34} and is denoted by $\mathcal{M}\{b_{24}, b_{34}\}$,where the b_{ij} take the values $(4-2n)/n$ in the i th and j th rows and $4/n$ elsewhere. The intersection of $\mathcal{M}\{\beta_{12}, \beta_{13}\}$ and $\mathcal{M}\{\beta_{24}, \beta_{34}\}$ is given by $c(b_{12} - b_{13})$ for arbitrary c, which is the same as $c(b_{24} - b_{34})$. Assuming for simplicity the error free case the projection of the component of the observation vector orthogonal to the mean and main effects, $ABb_{12} + ACb_{13}$, onto $b_{12} - b_{13}$ is given by $(AB - AC)(b_{12} - b_{13})/2$. The fitted false model component orthogonal to the mean and main effects is given by the vector $(AB - AC)(b_{12} - b_{13})/2$ plus the projection of $(ABb_{12} + ACb_{13} - (AB - AC)(b_{12} - b_{13})/2)$ onto $(b_{24} + b_{34})$ since $(b_{24} + b_{34})$ is obviously orthogonal to $(b_{24} - b_{34})$. Then $RSS^{1/2} = (AB + AC)||(b_{12} + b_{13})||(\sin\theta)/2$ where θ is the angle formed by $(b_{12} + b_{13})$ and $(b_{24} + b_{34})$. Hence

$$RSS = \frac{1}{4}(AB + AC)^2||(b_{12} + b_{13})||^2(1 - \cos^2\theta)$$

where

$$\cos\theta = \frac{(b_{12} + b_{13}) \cdot (b_{24} + b_{34})}{(||b_{12} + b_{13}||)(||b_{24} + b_{34}||)}$$

and evaluating this, and since the degrees of freedom is $(n - 3)$, we obtain

$$MSE = \frac{32(n-4)(AB + AC)^2}{(3n - 8)(n - 3)}.$$

Since the modified one-factor-at-a-time foldover design is symmetric in all the factors, the results in Table 3 also apply when factor labels are interchanged. For example, taking $n = 5$ and interchanging B with D and C with E, we can see that if $AD = -AE$ for the true model $\{AD, AE\}$ then the falso models $\{BD, BE\}$ and $\{CD, CE\}$ will also have $E(MSE) = \sigma^2$, agreeing with the example covered in the previous section.

The results in table 3 can be used in a number of ways. For example, assume that there exists a good estimate of the standard deviation σ. Then the standardized residual sum of squares (RSS/σ^2) follows a noncentral chi-square distribution with noncentrality parameter

$$\lambda = \beta_1' X_{1\cdot 0}'(I - X_{2\cdot 0}(X_{2\cdot 0}' X_{2\cdot 0})^{-1} X_{2\cdot 0}') X_{1\cdot 0}\beta_1.$$

The noncentrality parameter is of course zero for the true model. For each model we can calculate the RSS and separate those models that agree with the data from those that do not using the following method: For each competing model calculate (RSS/σ^2). If this value is less than the 95th percentile of a central chi-square distribution with the appropriate degrees of freedom then the model is considered *consonant* with the true model. Obviously the true model has a 0.05 probability of being labelled non-consonant, while the probability should be greater than or equal to 0.05 for each of the false models.

Number of factors , n	h
5	1.84
6	1.64
7	1.59
8	1.57
9	1.57

Table 4: Values of h such that $| AB + AC | \leq h\sigma$ forms a 95% consonance region for $\{BD, CD\}$.

For a particular false model M_2, a set of values of the true model parameters β_1 can be calculated for which the probability of declaring M_2 consonant with M_1 is greater than 0.05. We will call such a set a 95% consonance region for M_2. The region is calculated by setting λ so that

$$\Pr(\chi^2(\nu;\lambda) < {\chi^2}_{.95}(\nu)) = 0.05$$

where $\chi(\nu;\lambda)$ stands for the noncentral chi-square distribution with degrees of freedom ν and noncentrality parameter λ, ν = error degrees of freedom for model M_2, and ${\chi^2}_{\alpha}(\nu)$ stands for the 100α percentile of the central χ^2 distribution with degrees of freedom ν.

With M_1 given by $\{AB, AC\}$ and M_2 given by $\{BD, CD\}$ the consonance regions are of the form $| AB + AC | \leq h\sigma$. Table 4 gives the values of h for the modified one-factor-at-a-time foldover design with $5 \leq n \leq 9$. If the values of the two-factor interactions fall outside the consonance region then the probability that the false model can be separated from the true model on the basis of the data will be more than 0.95.

4. The Design of Augmenting runs

Daniel (1962;1976 Chap.14) discussed the design of augmenting trials to determine the real two-factor interactions in a significant two-factor interaction string arising from a two-level resolution IV design. We can use a similar idea following the use of a modified one-factor-at-a-time foldover design to determine which one of the competing models that cannot be separated on the basis of the data is the true model. The designs considered here can also be viewed as examples of "Probing designs" introduced by Srivastava(1989). The emphasis here, however, is quite different in that we deal only with the class of modified-one-factor-at-a-time foldover designs, both the error-free and error cases are covered as is the case when a block term is required.

It suffices to consider only one case in detail corresponding to the n factor design in $2n$ runs when the two non-zero interactions have one letter in common and opposite effects. We will initially assume the error-free case and without loss of generality relabel the factors so that the i th of the $(n-2)$ competing models consists of the interaction between the i th and $(n-1)$ th factors and the interaction between the i th and the n th factors, $1 \leq i \leq (n-2)$.

For the interaction between the k th and the l th factors $(1 \leq k < l \leq n)$ the corresponding column in the initial design, orthogonal to the mean, is b_{kl} and for the augmenting design B_{kl}. Both b_{kl} and B_{kl} take the value $(4/n)$ in rows where factors k and l take the same levels, and the values $(4-2n)/n$ elsewhere.

In order to separate the i th and j th model $(1 \leq i < j \leq (n-2))$ the column vector

$$C_{ij} = B_{i(n-1)} - B_{in} - B_{j(n-1)} + B_{jn}$$

must not be equal to $\mathbf{0}$, and hence for the augmenting design to be effective all the C_{ij} must not equal $\mathbf{0}$. Furthermore, if a block effect needs to be allowed for, which is most often the case in industrial experimentation, then the C_{ij} must not be proportional to the unit vector.

Note that

$$\begin{aligned} C_{1j} - C_{1i} &= B_{1(n-1)} - B_{1n} - B_{j(n-1)} + B_{jn} \\ &- [B_{1(n-1)} - B_{1n} - B_{i(n-1)} + B_{i(n)}] \end{aligned}$$

which equals C_{ij}. Moreover $C_{ij} = 0$ if and only if $C_{1j} = C_{1i}$, and $C_{ij} = x\mathbf{1}$ if and only if $C_{1j} = C_{1i} + x\mathbf{1}$, that is they differ by a constant amount.

Hence we need only examine the matrix

$$C = (C_{12}, C_{13}, \ldots, C_{1(n-2)})$$

in order to determine if the augmenting design will separate the (n-2) competing models.

The elements of C_{ij} can only take the values $-4, 0$ or 4. The value -4 is taken when the sign sequence of the factors $i, j, (n-1)$ and n is $(+,-,-,+)$

or $(-,+,+,-)$, the value 4 is taken when the sign sequence is $(+,-,+,-)$ or $(-,+,-,+)$, and the value 0 taken otherwise. The r rows of the matrix C can be reordered so that the first $r_1 \leq r$ rows take only the values 0's and 4's, while the last $r_2 = r - r_1$ rows take only the values 0's and -4's, since only these two possibilities exist.

Since the elements in each row can only take two possible values and there are r rows, the number of distinct columns of C is 2^r. One of these columns consists of all 0's and hence $(n-3) \leq 2^r - 1$ or $r \geq \log_2(n-2)$, if a block effect does not have to be taken into account. Note also that one of the columns consists of all 0's in the first r_1 rows and -4's in the last r_2 rows, while another column consists all 4's in the first r_1 rows and 0's in the last r_2 rows. If a block effect needs to be allowed for only one of these columns can be used and hence $(n-3) \leq 2^r - 2$ or $r \geq \log_2(n-1)$.

These results indicate that a two run augmenting design will be sufficient in the error free case for a 5 factor experiment if a block effect is required and for a 6 factor experiment if a block effect is not required. If we have conducted a 9 factor experiment in 18 trials then only 3 augmenting runs will be required. This latter result is potentially important since with the usual orthogonal resolution IV fractional replicates an increase from 16 to 32 trials is required when the number of factors increases from 8 to 9.

The use of the augmenting runs is illustrated with the reactor data example considered earlier. If we choose the matrix

$$C = \begin{pmatrix} 4 & 4 \\ -4 & 0 \end{pmatrix}$$

then, from examination of the corresponding sign sequences, the first run can be chosen to be *ad* and the second run to be *bd*. Using the corresponding response yields of 94 and 61 for these two runs from the original 2^5 design, the competing models, including now a block term, were fitted to the 12 observations. Table 5 gives the residual mean squares for the three competing models.

Clearly, in this case, the augmenting trials have allowed the identification of $\{AD, AE\}$ as the correct model. Of the 231 possible pairs of augmenting trials, 24 give eligible C matrices. The 24 pairs consist of any two runs from the set $\{ad, bd, cd\}$ or any two runs from the set $\{ae, be, ce\}$, where each of the selected runs can be exchanged for its foldover. Since a block term is fitted, the separation of the competing models depends only on the difference between the responses of the augmenting runs and hence, when error is present, we prefer the 12 pairs where only two factors change levels,

Interactions in model	MSE
$\{CD, CE\}$	33.30
$\{AD, AE\}$	8.35
$\{BD, BE\}$	147.19

Table 5: Mean square errors for the three competing models after the addition of the two augmenting runs *ad* and *bd*.

True Model	Δ/σ							
	0	0.5	1	1.5	2	2.5	3	3.5
$\{AD, AE\}$	13	84	438	792	929	957	960	952
$\{BD, BE\}$	15	104	433	779	933	937	948	948
$\{CD, CE\}$	9	5	61	431	833	951	939	964

Table 6: The number of simulations out of 1000 where the correct true model was identified, when the first two-factor interaction effect in the true model had a value of Δ and the second two-factor interaction effect had a value of $-\Delta$, following the addition of the augmenting runs *ad* and *bd*.

such as $\{ad, bd\}$ and $\{bce, ace\}$, rather than the 12 pairs where three factors change levels, such as $\{ad, ace\}$ and $\{bd, bce\}$.

If σ is known to be 3.5, then for models to be regarded as consonant with the true model the MSE needs to be less than 31.9. Of the 12 pairs of eligible augmenting runs with only two factors changing levels, 10 would have successfully identified $\{AD, AE\}$ as the true model. The success of this separation depends on the parameter values of the real two-factor interactions, the value of the standard deviation and also on which model is actually the true one. For example, for $\{ad, bd\}$ the separation will be less clear if $\{CD, CE\}$ turns out to be the true model. This is demonstrated by the simulation summarized in Table 6 giving, for various values of Δ/σ, the number of simulations out of 1000 where the correct true Model was identified, when one of the real two-factor interaction effects had a value of Δ and the other had a value of $-\Delta$. If the models are not separated after the initial augmenting runs then a further augmenting pair, giving less separation if either $\{AD, AE\}$ or $\{BD, BE\}$ are the true models, should be chosen.

5. Conclusion

The orthogonal resolution IV fractional replicates yield the most efficient estimates of the main effects and are relatively simple to design and analyse. However in most cases the two-factor interactions are aliased in strings, and if one or more of these strings are significant then augmenting trials will be required.

The designs considered in this paper involve a small sacrifice in the efficiency of the estimation of the main effects. The major advantages are the fewer number of runs required and the ability to identify and estimate a small number of real two-factor interactions as long as the two-factor interactions do not take certain values. Even if they do, then it is possible to design an augmenting set, involving only two trials with up to five factors and three trials with up to nine factors that will enable the identification and estimation to be done.

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