
Alternatives to resolution IV screening designs in 16 runs

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Abstract: The resolution IV regular fractional factorial designs in 16 runs for six, seven, and eight factors are in standard use. They are economical and provide clear estimates of main effects when three-factor and higher-order interactions are negligible. However, because the two-factor interactions are completely confounded, experimenters are frequently required to augment the original fraction with new runs to resolve ambiguities in interpretation. We identify non-regular orthogonal fractions in 16 runs for these situations that have no complete confounding of two-factor interactions. These designs allow for the unambiguous estimation of models containing both main effects and a few two-factor interactions. We present the rationale behind the selection of these designs from the non-isomorphic 16-run fractions and illustrate how to use them with an example from the literature.

Keywords: screening experiments; design resolution; aliases; non-regular designs.

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1 Introduction

Two-level fractional factorial designs are a staple for factor screening in industrial applications. Resolution IV designs are particularly popular because they avoid the confounding of main effects and two-factor interactions found in resolution III designs while avoiding the larger sample size requirements of resolution V designs. The minimum aberration versions of these designs are found by using the following generators: for six factors, $E = \pm ABC$ and $F = \pm BCD$; for seven factors, $E = \pm ABC$, $F = \pm BCD$, and $G = \pm ACD$; and for eight factors, $E = \pm BCD$, $F = \pm ACD$, $G = \pm ABC$, and $H = \pm ABD$. These designs have two-factor interactions that are completely confounded in seven alias chains.

The two-factor interaction aliasing in these designs can result in projects with ambiguous conclusions. For example, Montgomery (2009) presents a 2^{6-2} design used in a photoresist application process where four main effects A, B, C, and E are found to be important along with one two-factor interaction alias chain $AB + CE$. Without external process knowledge, the experimenter cannot decide whether the AB interaction, the CE interaction or some linear combination of them represents the true state of nature. To resolve this ambiguity requires additional runs.

While strong two-factor interactions may be less likely than strong main effects, there are many more interactions than main effects in screening situation. As a result, the likelihood of at least one significant interaction effect is quite high. There is often substantial institutional reluctance to commit additional time and material to a study with unclear results. Consequently, experimenters would like to avoid the need to plead for a follow-up study. We show how to lower the risk of analytical ambiguity by using a specific orthogonal but non-regular fractional factorial design. Our proposed designs for six, seven, and eight factor studies in 16 runs have no complete confounding of pairs of two-factor interactions. We prefer these designs and recommend them as alternatives for the usual regular minimum aberration resolution IV fractional factorials. In subsequent sections, we present a metric to evaluate these fractional factorial designs, use it to obtain our choices for the non-regular 16-run fractional factorials, and present an example that illustrates their usefulness.

2 Literature review

Plackett and Burman (1946) introduced non-regular orthogonal designs for sample sizes that are a multiple of four but not powers of two. Hall (1961) identified five non-isomorphic orthogonal designs for 15 factors in 16 runs. Our proposed six through eight factor designs are projections of the Hall designs created by selecting specific sets of columns. Contemporaneously with Hall's work, Box and Hunter (1961) introduced the regular fractional factorial designs that became the standard tools for factor screening. Sun et al. (2002) catalogued all the non-isomorphic projections of the Hall designs. Li et al. (2003) used this catalogue to identify the best designs to use in case there is a need for a foldover. For each of these designs they provide the columns to use for folding and the resulting resolution of the combined design. Loeppky et al. (2007) also used this catalogue to identify the best designs to use assuming that a small number of factors are active and the experimenter wished to fit a model including the active main effects and all two-factor interactions involving factors having active main effects.

3 Metrics for comparison of screening designs

Screening designs are primarily concerned with the discovery of active factors. This factor activity generally expresses itself through a main effect or a factor's involvement in a two-factor interaction. Consider the model,

$$y = \mathbf{X} \boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

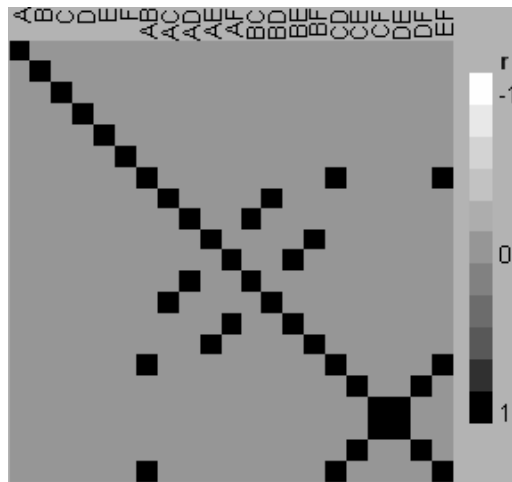
where \mathbf{X} contains columns for the intercept, main effects and all two-factor interactions, $\boldsymbol{\beta}$ is the vector of model parameters, and $\boldsymbol{\varepsilon}$ is the usual vector of $NID(0, \sigma^2)$. For six through eight factors in 16 runs, the matrix, \mathbf{X} has more columns than rows. Thus, it is not of full rank and the usual least squares estimate for $\boldsymbol{\beta}$ does not exist because the matrix $\mathbf{X}'\mathbf{X}$ is singular. With respect to this model, every 16 run design is supersaturated. Booth and Cox (1962) introduced the $E(s^2)$ criterion as a diagnostic measure for comparing supersaturated designs:

$$E(s^2) = \frac{1}{2} \sum_{i < j} (x_i'x_j)^2 / (k(k-1))$$

where k is the number of columns in \mathbf{X} .

Minimising the $E(s^2)$ criterion is equivalent to minimising the sum of squared off-diagonal elements of the correlation matrix of \mathbf{X} . Removing the constant column from \mathbf{X} , the correlation matrix of the regular resolution IV 16-run six-factor design is 21×21 with one row and column for each of the six main effects and 15 two-factor interactions. Figure 1 shows the correlation matrix for the principal fraction of this design. In Figure 1, we note that the correlation is zero between all main effects and two-factor interactions (because the design is resolution IV) and that the correlation is +1 between every two-factor interaction and at least one other two-factor interaction. These two-factor interactions are completely confounded. If another member of the same design family had been used at least one of the generators would have been used with a negative sign in design construction and some of the entries of the correlation matrix would have been -1. There still would be complete confounding of two-factor interactions in the design.

Figure 1 The correlation matrix for the regular 2^{6-2} resolution IV fractional factorial design



The cell plot of the correlation matrix is a useful graphical way to compare the non-regular designs that we propose to their regular fractional factorial counterparts. In Figure 1, it is a display of the confounding pattern. The alias matrix is a generalisation of the confounding pattern that is useful for comparing non-regular designs. Suppose that we plan to fit the model

$$y = \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\varepsilon}$$

where \mathbf{X}_1 is the design matrix for the experiment that has been conducted expanded to model form, $\boldsymbol{\beta}_1$ is the vector of model parameters, and $\boldsymbol{\varepsilon}$ is the usual vector of $NID(0, \sigma^2)$ errors but that the true model is

$$y = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon}$$

where the columns of \mathbf{X}_2 contain additional factors not included in the original model (such as interactions) and $\boldsymbol{\beta}_2$ is the corresponding vector of model parameters. It is straightforward to show that the expected value of $\hat{\boldsymbol{\beta}}_1$, the least squares estimate of $\boldsymbol{\beta}_1$, is

$$E(\hat{\boldsymbol{\beta}}_1) = \boldsymbol{\beta}_1 + (\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{X}'_1\mathbf{X}_2\boldsymbol{\beta}_2 = \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2$$

The alias matrix $\mathbf{A} = (\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{X}'_1\mathbf{X}_2$ shows how estimates of terms in the fitted model are biased by active terms that are not in the fitted model. Each row of \mathbf{A} is associated with a parameter in the fitted model. Non-zero elements in a row of \mathbf{A} show the degree of biasing of the fitted model parameter due to terms associated with the columns of \mathbf{X}_2 .

In a regular design, an arbitrary entry in the alias matrix, A_{ij} , is either 0 or ± 1 . If A_{ij} is 0 then the i th column of \mathbf{X}_1 is orthogonal to the j th column of \mathbf{X}_2 . Otherwise if A_{ij} is ± 1 , then the i th column of \mathbf{X}_1 and the j th column of \mathbf{X}_2 are perfectly correlated.

For non-regular designs the aliasing is more complex. If \mathbf{X}_1 is the design matrix for the main effects model and \mathbf{X}_2 is the design matrix for the two-factor interactions, then the entries of the alias matrix for orthogonal non-regular designs for 16 runs take the values 0, ± 1 or ± 0.5 . A small subset of these designs have no entries of ± 1 .

Bursztyrn and Steinberg (2006) propose using the trace of $\mathbf{A}\mathbf{A}'$ as a scalar measure of the total bias in a design. They use this as a means for comparing designs for computer simulations but this measure works equally well for ranking competitive screening designs.

4 The proposed designs and their properties

Table 1 shows the number of non-isomorphic orthogonal 16 run designs. By non-isomorphic, we mean that one cannot obtain one of these designs from another one by permuting the rows or columns or by changing the labels of the factor.

Table 1 Number of 16-run orthogonal non-isomorphic designs

<i>Number of factors</i>	<i>Number of designs</i>
6	27
7	55
8	80

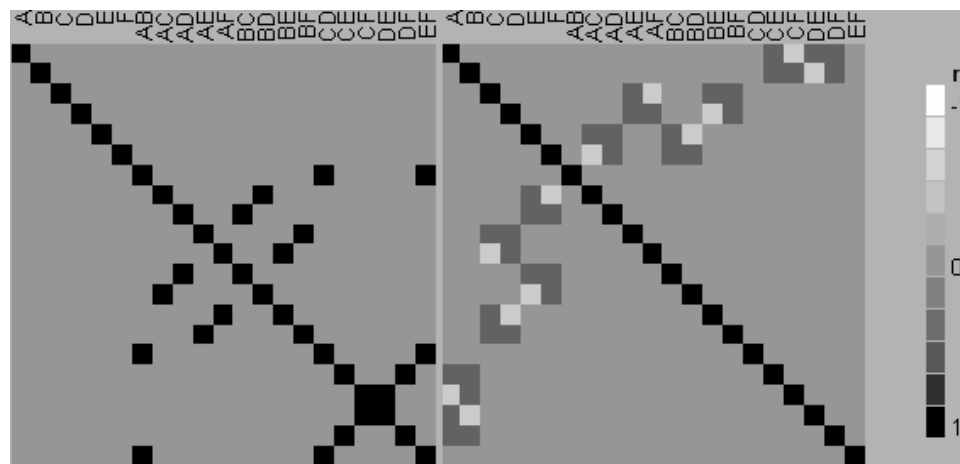
The non-regular designs that we recommend are selected from the designs represented in Table 1. We first present our recommendations and then discuss their properties and our reasons for selecting them as alternatives to the usual resolution IV designs.

For six factors, our recommended design is in Table 2. The correlation matrix for this design along with the correlation matrix for the regular fraction is in Figure 2.

Table 2 Recommended 16-run six-factor no-confounding design

Run	A	B	C	D	E	F
1	1	1	1	1	1	1
2	1	1	-1	-1	-1	-1
3	-1	-1	1	1	-1	-1
4	-1	-1	-1	-1	1	1
5	1	1	1	-1	1	-1
6	1	1	-1	1	-1	1
7	-1	-1	1	-1	-1	1
8	-1	-1	-1	1	1	-1
9	1	-1	1	1	1	-1
10	1	-1	-1	-1	-1	1
11	-1	1	1	1	-1	1
12	-1	1	-1	-1	1	-1
13	1	-1	1	-1	-1	-1
14	1	-1	-1	1	1	1
15	-1	1	1	-1	1	1
16	-1	1	-1	1	-1	-1

Figure 2 Correlation matrix (a) regular 2^{6-2} fractional factorial (b) the no-confounding design



Notice that like the regular 2^{6-2} the proposed design is orthogonal but unlike the regular design, there are no two-factor interactions that are aliased with each other. All of the off-diagonal entries in the correlation matrix are between -1 and $+1$. Because there is no complete confounding of two-factor interactions, we call this a no-confounding design.

Table 3 presents the recommended seven-factor 16-run design. The correlation matrix for this design and the regular 2^{7-3} fraction is shown in Figure 3. The no-confounding design is orthogonal and there is no complete confounding of two-factor interactions.

Table 3 Recommended 16-run seven factor no-confounding design

Run	A	B	C	D	E	F	G
1	1	1	1	1	1	1	1
2	1	1	1	-1	-1	-1	-1
3	1	1	-1	1	1	-1	-1
4	1	1	-1	-1	-1	1	1
5	1	-1	1	1	-1	1	-1
6	1	-1	1	-1	1	-1	1
7	1	-1	-1	1	-1	-1	1
8	1	-1	-1	-1	1	1	-1
9	-1	1	1	1	1	1	-1
10	-1	1	1	-1	-1	-1	1
11	-1	1	-1	1	-1	1	1
12	-1	1	-1	-1	1	-1	-1
13	-1	-1	1	1	-1	-1	-1
14	-1	-1	1	-1	1	1	1
15	-1	-1	-1	1	1	-1	1
16	-1	-1	-1	-1	-1	1	-1

Figure 3 Correlation matrix (a) regular 2^{7-3} fractional factorial (b) the no-confounding design

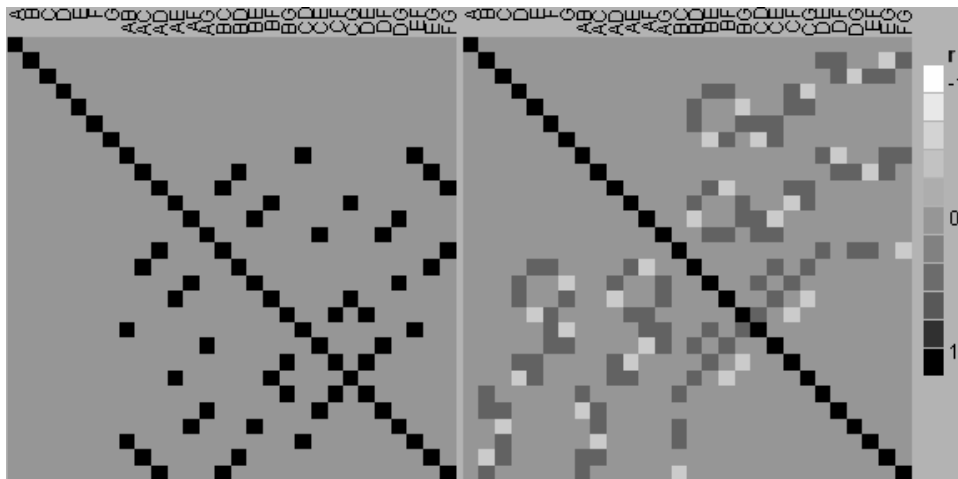


Table 4 presents the recommended eight-factor 16-run design. The correlation matrix for this design and the regular 2^{8-4} fraction is shown in Figure 4. The no-confounding design is orthogonal and there is no complete confounding of two-factor interactions.

Table 4 Recommended 16-run eight factor no-confounding design

Run	A	B	C	D	E	F	G	H
1	1	1	1	1	1	1	1	1
2	1	1	1	1	-1	-1	-1	-1
3	1	1	-1	-1	1	1	-1	-1
4	1	1	-1	-1	-1	-1	1	1
5	1	-1	1	-1	1	-1	1	-1
6	1	-1	1	-1	-1	1	-1	1
7	1	-1	-1	1	1	-1	-1	1
8	1	-1	-1	1	-1	1	1	-1
9	-1	1	1	1	1	1	1	1
10	-1	1	1	-1	1	-1	-1	-1
11	-1	1	-1	1	-1	-1	1	-1
12	-1	1	-1	-1	-1	1	-1	1
13	-1	-1	1	1	-1	-1	-1	1
14	-1	-1	1	-1	-1	1	1	-1
15	-1	-1	-1	1	1	1	-1	-1
16	-1	-1	-1	-1	1	-1	1	1

Figure 4 Correlation matrix (a) regular 2^{8-4} fractional factorial (b) the no-confounding design

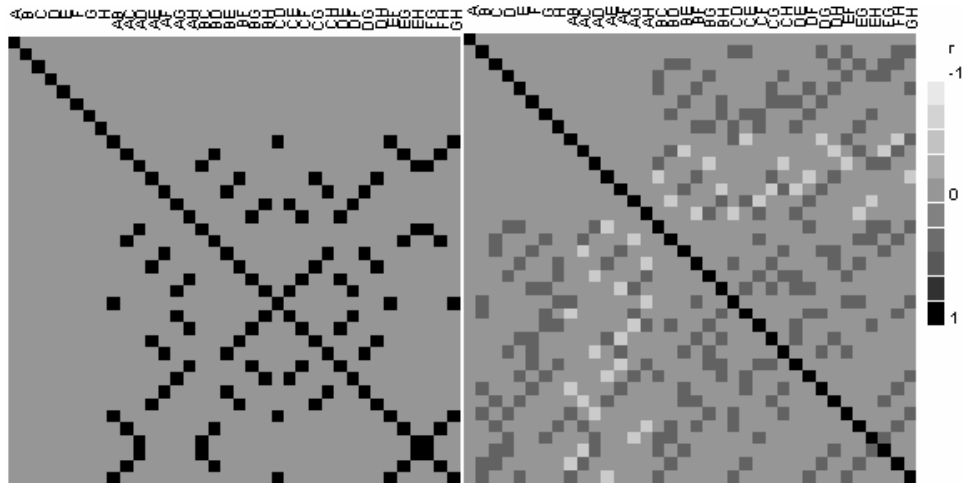


Table 5 compares the popular minimum aberration resolution IV designs to our recommended designs on the metrics described in the previous section.

Table 5 Design comparison on metrics

<i>N factors</i>	<i>Design</i>	<i>Confounded effect pairs</i>	<i>E(s²)</i>	<i>Trace(AA')</i>
6	Recommended	0	7.31	6
	Resolution IV	9	10.97	0
7	Recommended	0	10.16	6
	Resolution IV	21	14.20	0
8	Recommended	0	12.80	10.5
	Resolution IV	42	17.07	0

As shown in the cell plots of the correlation matrices, the recommended designs outperform the minimum aberration designs for the number of confounded pairs of effects. They also are substantially better with respect to the $E(s^2)$ criterion. The price that our recommended designs pay for avoiding any pure confounding is that there is some correlation between main effects and two-factor interactions as shown in the last column.

5 Example

Montgomery (2009) presents an example of the regular 2^{6-2} resolution IV design applied to a photoresist application process. The response variable is thickness and the design factors are A = speed RPM, B = acceleration, C = volume, D = time, E = resist viscosity, and F = exhaust rate. Table 6 shows the design.

Table 6 Photoresist experiment (2^{6-2})

<i>Run</i>	<i>A</i>	<i>B</i>	<i>C</i>	<i>D</i>	<i>E</i>	<i>F</i>	<i>Thickness</i>
1	-1	-1	-1	-1	-1	-1	4,524
2	1	-1	-1	-1	1	-1	4,657
3	-1	1	-1	-1	1	1	4,293
4	1	1	-1	-1	-1	1	4,516
5	-1	-1	1	-1	1	1	4,508
6	1	-1	1	-1	-1	1	4,432
7	-1	1	1	-1	-1	-1	4,197
8	1	1	1	-1	1	-1	4,515
9	-1	-1	-1	1	-1	1	4,521
10	1	-1	-1	1	1	1	4,610
11	-1	1	-1	1	1	-1	4,295
12	1	1	-1	1	-1	-1	4,560
13	-1	-1	1	1	1	-1	4,487
14	1	-1	1	1	-1	-1	4,585
15	-1	1	1	1	-1	1	4,195
16	1	1	1	1	1	1	4,510

Source: From Montgomery (2009)

Table 7 shows the output from the JMP screening analysis for this experiment. From the analysis, we conclude that the main effects of factors A, B, C, and E are important and that the two-factor interaction alias chain AB + CE is important. Because AB and CE are completely confounded, either additional information or assumptions are necessary to avoid analytical ambiguity.

Table 7 JMP screening analysis for the photoresist experiment in Table 6

<i>Term</i>	<i>Contrast</i>	<i>Length t-ratio</i>	<i>p-value</i>	<i>Aliases</i>
A	85.3125	6.11	0.0007*	B*C*E, E*F*D
B	-77.6875	-5.56	0.0014*	A*C*E, C*F*D
C	-34.1875	-2.45	0.0309*	A*B*E, B*F*D
E	21.5625	1.54	0.1298	A*B*C, A*F*D
F	-14.6875	-1.05	0.2690	B*C*D, A*E*D
D	7.5625	0.54	0.6158	B*C*F, A*E*F
A*B	54.8125	3.92	0.0074*	C*E
A*C	-3.4375	-0.25	0.8175	B*E
B*C	3.3125	0.24	0.8242	A*E, F*D
A*F	-16.4375	-1.18	0.2231	E*D
B*F	8.0625	0.58	0.5900	C*D
C*F	-2.6875	-0.19	0.8563	B*D
E*F	10.5625	0.76	0.4166	A*D
A*B*F	10.8125	0.77	0.4065	C*E*F, A*C*D, B*E*D
A*C*F	-5.6875	-0.41	0.7028	B*E*F, A*B*D, C*E*D

We now consider an alternative experimental design for this problem, the no-confounding six-variable design from Table 2. Table 8 presents this design with a set of simulated response data for the injection moulding experiment. In constructing the simulation, we assumed that the main effects that were important were A, B, C, and E. We also assumed the CE interaction was the true source of the AB + CE effect observed in the actual study. We added normal random noise in our simulated data to match the RMSE of the fitted model in the original data. We also matched that the model parameter estimates to those from the original experiment. Our intent was to create a fair realisation of the data that might have been observed if the no-confounding design had been used.

Table 8 The no-confounding design for the photoresist application experiment

<i>Run</i>	<i>A</i>	<i>B</i>	<i>C</i>	<i>D</i>	<i>E</i>	<i>F</i>	<i>Thickness</i>
1	1	1	1	1	1	1	4,494
2	1	1	-1	-1	-1	-1	4,592
3	-1	-1	1	1	-1	-1	4,357
4	-1	-1	-1	-1	1	1	4,489
5	1	1	1	-1	1	-1	4,513
6	1	1	-1	1	-1	1	4,483
7	-1	-1	1	-1	-1	1	4,288

Table 8 The no-confounding design for the photoresist application experiment (continued)

<i>Run</i>	<i>A</i>	<i>B</i>	<i>C</i>	<i>D</i>	<i>E</i>	<i>F</i>	<i>Thickness</i>
8	-1	-1	-1	1	1	-1	4,448
9	1	-1	1	1	1	-1	4,691
10	1	-1	-1	-1	-1	1	4,671
11	-1	1	1	1	-1	1	4,219
12	-1	1	-1	-1	1	-1	4,271
13	1	-1	1	-1	-1	-1	4,530
14	1	-1	-1	1	1	1	4,632
15	-1	1	1	-1	1	1	4,337
16	-1	1	-1	1	-1	-1	4,391

We analysed this experiment using forward stepwise regression with all main effect and two-factor interactions as candidate effects. The reason that all two-factor interactions can be considered as candidate effects is that none of these interactions are completely confounded. The JMP stepwise regression output is in Figure 9.

Table 9 JMP stepwise regression output for the no-confounding design in Table 8

<i>Lock</i>	<i>Entered</i>	<i>Parameter</i>	<i>Estimate</i>	<i>nDF</i>	<i>SS</i>	<i>'F Ratio'</i>	<i>'Prob>F'</i>
X	X	Intercept	4,462.8125	1	0	0.000	1
	X	A	85.3125	1	77,634.37	53.976	2.46e-5
	X	B	-77.6825	1	64,368.76	44.753	5.43e-5
	X	C	-34.1875	2	42,735.84	14.856	0.00101
		D	0	1	31.19857	0.020	0.89184
	X	E	21.5625	2	31474.34	10.941	0.00304
		F	0	1	2,024.045	1.474	0.25562
		A*B	0	1	395.8518	0.255	0.6259
		A*C	0	1	476.1781	0.308	0.59234
		A*D	0	2	3,601.749	1.336	0.31571
		A*E	0	1	119.4661	0.075	0.78986
		A*F	0	2	4,961.283	2.106	0.18413
		B*C	0	1	60.91511	0.038	0.84923
		B*D	0	2	938.8809	0.279	0.76337
		B*E	0	1	3,677.931	3.092	0.11254
		B*F	0	2	2,044.119	0.663	0.54164
		C*D	0	2	1,655.264	0.520	0.61321
	X	C*E	54.8125	1	2,4035.28	16.711	0.00219
		C*F	0	2	2,072.497	0.673	0.53667
		D*E	0	2	79.65054	0.022	0.97803
		D*F	0	0	0		
		E*F	0	2	5,511.275	2.485	0.14476

Notice that stepwise regression selects the main effects of A, B, C, E, along with the CE interaction. The no-confounding design correctly identifies the model unambiguously and without requiring additional runs.

6 Concluding remarks

We have presented no-confounding designs for the cases of 16 runs and six, seven or eight factors. We propose these as alternatives to the usual 16-run regular resolution IV minimum aberration fractions. These are non-regular orthogonal designs that avoid any pure confounding of main effects with two-factor interactions or two-factor interactions with each other. For all the non-isomorphic orthogonal designs for six, seven or eight factors, these designs minimise the $E(s^2)$ criterion for a supersaturated model containing all the main effects and two-factor interactions. For each of our recommended designs the majority of effects are uncorrelated. The largest magnitude correlation of any effect with any other effect is one half. This compares favourably to resolution IV designs where groups of two-factor interactions have correlations of one or negative one making them individually unresolvable.

The regular six, seven and eight factor designs in 16 runs are widely used in practice because they are economical and they provide good information on main effects with the ability to detect active alias sets of two-factor interactions. However, due to this complete confounding of two-factor interactions, experimenters without strong prior engineering knowledge need to augment these designs to resolve ambiguities whenever one of these aliased sets of two-factor interactions is active. The non-regular no-confounding designs that we propose can be analysed using stepwise regression or other model selection techniques. These designs can correctly identify the underlying model for any number of main effects and a small number of two-factor interactions without additional runs. We therefore prefer them to resolution IV regular fractional factorial designs and recommend their standard use.

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