Constructing 2-level Fold-over Designs with Minimal Aliasing

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Abstract

This paper introduces three algorithms for constructing 2-level foldover designs using the G_2-aberration criterion (Tang & Deng, 1999). Our algorithms can find designs with the fully aliased 2-factor interactions (2FIs) eliminated. As a result, follow-up runs which are used to isolate the 2FI from another might become unnecessary. The constructed designs are compared with the efficient 2-level fold-over designs of Errore et al. (2017), the 2-level designs of strength 3 for 32, 40 and 48 runs of Schoen & Mee (2012), and some regular fractional factorial designs for up to 64 runs in the literature. A catalogue of G_2-aberration 2-level fold-over designs for up to 32 factors is given.

Keywords: Fractional factorial designs; Interchange algorithm; Coordinate-exchange algorithm; Non-orthogonal designs; Strength-3 orthogonal arrays; Screening Designs.

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1 Introduction

In the experiment to study the Chlofibric acid synthesis (Phan-Tan-Luu & Mathieu, 2000), the response measured was the reaction yield. The seven 2-level factors studied are: (1) Solution C addition temperature (25^{o}C and 45^{o}C); (2) Solution B addition temperature (25^{o}C and 45^{o}C); (3) Stirring duration of the reactional medium before the addition of solution B (5min and 60min); (4) Solution B addition duration (30min and 60 min); (5) Ratio NaOH/C (4 and 5.6); (6) Ratio B/C (1 and 1.5); and (7) Soda nature (Pearl and Pastille). The design for this experiment is a 2^{7-3}_{IV}, a fractional factorial design (FFD) of resolution IV, with the first four factors forming a factorial and the remaining factors are generated by the following design generators $7 = 123$, $5 = 134$ and $6 = 234$. This design can also be considered as a fold-over design (FOD) with eight runs as in Figure 1, forming the first half-fraction design (HFD) matrix. The other HFD matrix is obtained by reversing the signs of all columns of the original HFD matrix.

(1)	(2)	(3)	(4)	(5)	(6)	(7)
-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	-1	1	1	1	-1	-1
-1	1	1	1	-1	1	-1
1	1	1	1	1	1	1

Figure 1: HFD matrix of the Chlofibric acid synthesis experiment.

By construction, the main effects (MEs) of the design, whose HFD matrix is shown in Figure 1, are orthogonal to each other and to the 2-factor interactions (2FIs). However, the 2FIs pairs are aliased with each other: $12 = 37 = 56$, $13 = 27 = 45$, $14 = 35 = 67$, $15 = 26 = 34$, $16 = 25 = 47$, $17 = 23 = 45$ and $24 = 36 = 57$. Is there another design having the same number of factors and runs with no fully aliased 2FIs?

Errore et al. (2017), hereafter abbreviated as EJLN, point out four desirable features for screening designs, such as the one for the Chlofibric acid synthesis experiment: (i) orthogonality of MEs; (ii) orthogonality of MEs and 2FIs; (iii) orthogonality of 2FIs with one another and (iv) small run size. The Plackett-Burman designs and resolution III FFDs have features (i) and (iv) but not (ii) and (iii). The resolution IV FFDs, such as the one used in the Chlofibric acid synthesis experiment, have all desirable features except (iii). Finally, the resolution V FFDs have all desirable features except (iv). EJLN extended the work of Lin, Miller & Sitter (2008) and other authors on fold-over non-orthogonal designs, and introduced a new class of efficient 2-level FODs. EJLN-efficient FODs are available for m (the number of factors), ranging from 3 to 13, and the number of runs being equal to or greater than $2m$. Being FODs, these designs have MEs orthogonal to 2FIs. In addition, they can be constructed such that the fully aliased 2FIs can be eliminated.

The purposes of this paper are: (i) to introduce some algorithms for constructing FODs using the G_2-aberration criterion (Tang & Deng, 1999); (ii) to compare the constructed FODs with those of EJLN and the 2-level designs of strength 3 for 32, 40 and 48 runs in Schoen & Mee (2012), and some regular FFDs for up to 64 runs in the literature and (iii) to construct a catalogue of G_2-aberration FODs for up to 32 factors.

The book chapter of Phan-Tan-Luu & Mathieu (2000) and the book of Lewis et al. (1999) provide the necessary background knowledge for those working on chemical data on FFDs and related design concepts such as the Hadamard matrices, design resolution, confounding effects, fold-over designs, screening designs, etc. Examples on the use of the G_2-aberration and G-aberration criteria as design quality measures can be found in Ingram & Tang (2005), Schoen & Mee (2012), Schoen et al. (2017), Vazquez et al. (2019) and other authors.

2 Using G_2-aberration as a surrogate criterion for finding FODs

Consider a 2-level design, whose model includes the MEs and 2FIs, constructed from the $n \times m$ design matrix $\mathbf{D} = (d_{ui}),\ u = 1, \ldots, n;\ i = 1, \ldots, m$:

$$y_u = \beta_0 + \sum_{i=1}^{m} \beta_i d_{ui} + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij} d_{ui} d_{uj} + \epsilon_u \; u = 1, \ldots, n. \tag{1}$$

Here, y_u is the response at run u; β's are the unknown parameters; and ϵ_u (ϵ_u iid $\mathrm{N}(0, \sigma^2)$) is the error associated with run u. Note that the first $m+1$ terms in (1) form the ME model. In matrix notation, (1) can be written as $\mathbf{y} = \mathbf{X}\beta + \epsilon$, where $\mathbf{X}$ is the model matrix of size $n \times p$ with $p = 1 + m + \binom{m}{2}$. The uth row of $\mathbf{X}$ can be written as $(1,\ d_{u1}, \ldots,\ d_{um},\ d_{u1}d_{u2}, \ldots,\ d_{u(m-1)}d_{um})$. The information matrix $\mathbf{X}'\mathbf{X}$ contains the following elements: (i) $\sum d_i,\ (i = 1, \ldots, m)$; (ii) $\sum d_i d_j,\ (i < j)$; (iii) $\sum d_i d_j d_k,\ (i < j < k)$; and (iv) $\sum d_i d_j d_k d_l$ $(i < j < k < l)$, where $i,\ j,\ k,\ l = 1, \ldots, m$ and the summations are taken over n design points. The number of summations of the types (i), (ii), (iii) and (iv) are m, $\binom{m}{2}$, $\binom{m}{3}$ and $\binom{m}{4}$ respectively.

For regular FFDs - i.e. 2^{m-k} FFDs whose the first $m-k$ factors form a factorial and the remaining k factors are generated by k generators, like those in Table 12.15 of Box (1978) or Appendix G of Mee (2009) - the summations in (i)-(iv) are either 0 or $\pm n$. If all the summations of the types (i) and (ii) are zeros and at least one of the type (iii) is nonzero, it is called resolution III. If all the summations of the types (i)-(iii) are zeros and at least one of the type (iv) is nonzero, it is called resolution IV. Finally, if all the summations of the types (i)-(iv) are zeros, it is called resolution V. For non-regular FFDs which include non-orthogonal designs, the summations of the types (i)-(iv) can take a value between $-n$ and n. This means that, unlike regular FFDs in which any two effects are either orthogonal or fully aliased, non-regular FFDs might possess two effects that are partially aliased, i.e. they are neither orthogonal nor fully aliased.

We use $A_1,\ A_2,\ A_3$ and A_4 to denote the sums of squares of the summations of the types (i)-(iv) divided by n^2, respectively. For the regular FFD in the Introduction, readers can verify that all summations of the types (i), (ii) and (iii) are 0's. Of the 35 $(=\binom{7}{4})$ summations of the type (iv), the following seven summations $\sum d_1d_2d_3d_7 = \sum d_1d_2d_5d_6 = \sum d_1d_3d_4d_5 = \sum d_1d_4d_6d_7 = \sum d_2d_3d_4d_6 = \sum d_2d_4d_5d_7 = \sum d_3d_5d_6d_7 = 16$ and the remaining summations are 0's. The A_4 value of this FFD is $7 = (7 \times 16^2)/16^2$. For a regular FFD, A_4, called the number of length-4 words, is also a number producing full aliasing and each length-4 word defines three fully aliased 2FIs pairs. The first length-4 word 1237, for example, defines three fully aliased 2FIs pairs 12=37, 13=27 and 17=23.

As for a FOD (i.e. a design whose first HFD matrix is $\mathbf{D}$ and the second is $-\mathbf{D}$), its A's with odd subscripts will be zeros, and its A_2 and A_4 will be the same as $\mathbf{D}$. Our approach to using G_2-aberration criterion as a surrogate criterion for finding FODs is to find the most D-efficient design among the designs with the minimum $(A_2,\ A_4)$ pair. A FOD d^* constructed from the HFD matrix $\mathbf{D}^*$ (with A_2^* and A_4^*) is said to have less G_2 aberration (and to be more desirable) than a FOD d constructed from the HFD matrix $\mathbf{D}$ with A_2 and A_4 having the same number of factors and runs, when $A_2^* < A_2$, or $A_2^* = A_2$ and $A_4^* < A_4$.

Although the G_2 aberration criterion is computationally-cheap and popular, there is no guarantee that the most D-efficient FOD has the minimum $(A_2,\ A_4)$. At the same time, the most D-efficient design might not be the most desirable one. Note that sums of squares of the summations of the types (i)-(iv) are the sum of squares of the elements of $\mathbf{X'X}$, and minimizing them is equivalent to minimizing trace $(\mathbf{X'X})^2$ given a constant trace $(\mathbf{X'X})$. This is similar to the case of 2-level designs being the same as minimizing $\sum \lambda_i^2$ given a constant $\sum \lambda_i$, where $\lambda_1, \lambda_2, \ldots$ are the eigenvalues of $\mathbf{X'X}$. Clearly, smaller $\sum \lambda_i^2$ tends to give smaller $\sum \lambda_i^{-1}$ and larger $\Pi\lambda_i$, which are related to the well-known A- and D-optimality criteria, respectively.

3 The FOLD algorithms

In this section, we will describe three algorithms for constructing an HFD matrix $\mathbf{D}$ of size $n \times m$ $(m \leq n)$, from which a FOD for m factors in $2n$ runs can be constructed. For all three algorithms, we have to calculate A_2 and A_4. To calculate A_2 and A_4, we calculate vector J_u of length $\binom{m}{2} + \binom{m}{4}$ for each row u of $\mathbf{D}$, $(u = 1, \ldots, n)$:

$$J_u = (d_{u1}d_{u2}, \ldots,\ d_{u(m-1)}d_{um},\ d_{u1}d_{u2}d_{u3}d_{u4}, \ldots,\ d_{u(m-3)}d_{u(m-2)}d_{u(m-1)}d_{um}). \qquad (2)$$

We then calculate $J = \sum_{u=1}^{n} J_u$ and set A_2 and A_4 equal to the sums of squares of the first $\binom{m}{2}$ elements of J and the last $\binom{m}{4}$ elements of J divided by n^2 respectively.

(i) **FOLD**$_1$: **FOLD**$_1$ makes use of an input ± 1 matrix of order $n \geq m$. **FOLD**$_1$ picks a random sample of m distinct columns from the input matrix. Each sample makes up one "try". Among all tries which result in the minimum $(A_2,\ A_4)$ pair, we choose the one with the maximum D-efficiency defined as:

$$D_{\text{eff}} = \frac{1}{2n} |\mathbf{X}_1' \mathbf{X}_1|^{\frac{1}{m+1}} \tag{3}$$

where $\mathbf{X}_1$ is the model matrix corresponding to the intercept term and the linear MEs.

Remarks:

1. If $n = 4t$, where t is an integer, a chosen Hadamard matrix (Hedayat & Wallis, 1978) of order n is used as the input matrix. A ± 1 square matrix $\mathbf{H}$ of order n is Hadamard if $\mathbf{H}'\mathbf{H} = n\mathbf{I}$, where $\mathbf{I}$ is the identity matrix. Hadamard matrices of order up to $n = 256$ are available at `http://neilsloane.com/hadamard/`. If $n = 4t - 1$, the core of a normalized Hadamard matrix (a Hadamard matrix with all of the elements of the first row and first column are +1) of order $n + 1$ will be used.

2. **FOLD**$_1$ makes use of the Theorem 4.16 of Hedayat & Wallis (1978). This theorem states that if $\mathbf{H}$ is a semi-normalized Hadamard matrix (a Hadamard matrix with all of the elements of the first column are +1), using $\mathbf{H}$ as a HFD matrix will result in a strength-3 orthogonal array (OA). Also note that deleting the first column of this Hadamard matrix will result in a strength-2 OA.

(ii) **FOLD**$_2$: **FOLD**$_2$ and **FOLD**$_3$ are used when we want to construct a design from scratch, or when we want to add additional columns to m_0 columns of an HFD matrix. These two algorithms are also used to construct FODs with the fully aliased 2FIs pairs eliminated. Let $\max_2$ and $\max_4$ denote the maximum values (in terms of the absolute values) of the first $\binom{m}{2}$ and the last $\binom{m}{4}$ elements of J. When $\max_4$ becomes n, we understand that there are fully aliased 2FIs in the design. To eliminate these fully aliased 2FIs, we impose the condition $\max_4 < c$, where $c < n$, in selecting the candidate designs. The (column-wise) interchange algorithm $\mathbf{FOLD}_2$ is used when we wish to impose the equal-occurrence constraint (of $\pm$)upon each column of the HFD matrix $\mathbf{D}$ (each column has half of its elements at $+1$ and half at -1). $\mathbf{FOLD}_2$ has two steps:

1. Randomly allocate 1 to half of number of elements of columns j of $\mathbf{D}$ ($j = m_0 + 1, \ldots, m$), and -1 to the remaining elements. Calculate vector J and the $(A_2,\ A_4)$ pair.

2. For column j of $\mathbf{D}$ ($j = m_0 + 1, \ldots, m$), search for a pair of different elements such that swapping them results in the smallest pair $(A_2,\ A_4)$. If found, swap them and update $\mathbf{D}$ and J. Repeat this step until no further improvement on $(A_2,\ A_4)$ can be made.

For each parameter set $(m,\ n)$, Steps 1-2 make up one "try". Choose the one with the maximum D_{eff} among all tries which result in the minimum $(A_2,\ A_4)$ pair.

(iii) $\mathbf{FOLD}_3$: The coordinate-exchange algorithm $\mathbf{FOLD}_3$ is used when there is no need for us to impose the equal-occurrence constraint upon each column of the HFD matrix $\mathbf{D}$. Unlike FODs constructed by $\mathbf{FOLD}_1$ and $\mathbf{FOLD}_2$, designs constructed by $\mathbf{FOLD}_3$ cannot be blocked into two orthogonal blocks (using the first HFD matrix as the first block and the second half as the second block). The main difference between our implementation of the coordinate-exchange algorithm and the one of EJLN is the use of the objective function. While EJLN used D_{eff} as the only design criterion, we use G_2 aberration as the surrogate criterion in addition to the D_{eff} one. $\mathbf{FOLD}_3$ has two steps:

1. Randomly allocate ± 1 to elements of columns j of $\mathbf{D}$ ($j = m_0 + 1, \ldots, m$). Calculate vector J and the $(A_2,\ A_4)$ pair.

2. For column j of $\mathbf{D}$ ($j = m_0 + 1, \ldots, m$), search for an element such that changing its sign of the value results in the smallest pair $(A_2,\ A_4)$. If found, change the sign of the value of this element and update $\mathbf{D}$ and J. Repeat this step until no further improvement on $(A_2,\ A_4)$ can be made.

For each parameter set $(m,\ n)$, Steps 1-2 make up one "try". Choose the one with the maximum D_{eff} among all tries which result in the minimum $(A_2,\ A_4)$ pair, .

4 Using FOLD algorithms to construct FODs with Minimal Aliasing

Table 1 displays the quality measures of 33 FODs with m ranging from 3 to 16 and run sizes $\geq 2m$ (Cf. Table 1 of EJLN). The quality measures of these selected FODs include: A_2, A_4, $\max_2$ (and the frequency of $\max_2$ in the first $\binom{m}{2}$ elements of J) , $\max_4$ (and the frequency of $\max_4$ in the last $\binom{m}{4}$ elements of J), r_{ave} and $r_{\max}$ (= $\max_2$/n) which are the average and the maximum of the correlations between the MEs (in terms of the absolute values), the design D-efficiency D_{eff} defined in (2) and df(2FI) which is the rank of $\mathbf{X}_2$, the model matrix for 2FIs (Schoen & Mee, 2012). Note that designs with $\max_4 = n$ in this table (those marked with an asterisk) indicate that they have fully aliased 2FIs. We use 1,000 tries for each parameter set in Table 1 and the whole table was constructed in about five minutes on a laptop with CORE$^{\text{TM}}$i7.

Out of 33 FODs in Table 1, 17 have $A_2 = r_{\text{ave}} = r_{\max} = 0$ and $D_{\text{eff}} = 1$. Of these 17, those with $n = 4$ and 8 are regular resolution IV FFD and those with $n = 12$ and 16 are strength-3 OAs as those constructed by Schoen & Mee (2012). The remaining designs are non-orthogonal FODs. Chapter 7 of Mee (2009) give detailed account of these three classes of designs. The HFD matrices of the FODs in Table 1 for $n = 4t$ or $n = 4t - 1$ were constructed by $\mathbf{FOLD}_1$ using Hadamard matrices and cores of the normalized Hadamard matrices, respectively. The Hadamard matrix of order 16 which was used to construct four designs for $(m,\ n)$= (13, 16), (14,16), (15,16) and (16, 16) was constructed by $\mathbf{FOLD}_2$. The remaining FODs were constructed by $\mathbf{FOLD}_3$.

Out of 27 FODs in Table 1 of EJLN, 18 match ours in terms of the D_{eff} measures. For five parameter sets $(m,\ n)$=(7, 7), (9, 11), (10, 11), (11,11) and (13, 15), the EJLN's FODs are slightly more D-efficient than ours. Our designs, however, satisfy the near equal-occurrence constraint for each column and as a result have less G_2-aberration than EJLN's.

For four parameter sets $(m,\ n)$=(9, 10), (10, 10), (13, 14) and (14, 14), the EJLN's FODs are also more D-efficient than ours. However, none of our FODs for these parameters sets have 2FIs pairs being fully aliased or close to fully aliased as as EJLN FODs. For the mentioned nine parameter sets, if we use the ± 1 maximal-determinant matrix of order n in `http://www.indiana.edu/~maxdet/` as input matrices, we will get the FODs with about the same D_{eff} as EJLN's.

FODs in Table 1 with $\max_4 = n$ have fully aliased 2FIs. Table 2 shows 16 non-orthogonal FODs with fully aliased 2FIs eliminated for $n = 8$ and 16. In this table, FODs were constructed using a pre-set value of $\max_4 < c$, where $c < n$. Each parameter set (m, n) in Table 2 has two solutions. Those with low $\max_2$ values have high $\max_4$ values and vice versa. FODs for $n = 16$ and $m = 10$-15 and $\max_4 = 8$ were constructed by $\mathbf{FOLD}_2$. As such, these designs satisfy the equal-occurrence constraint for each column. The remaining designs in Table 2 were constructed by either $\mathbf{FOLD}_3$ or $\mathbf{FOLD}_2$ with the equal-occurrence constraint for each column relaxed.

Figure 2 shows two HFD matrices of two minimal aliased FODs for $(m,\ n)$ =(7, 8): (a) the one with $\max_2 = \max_4 = 4$ and (b) the one with $\max_2 = 2$ and $\max_4 = 6$. Both FODs have the same D_{eff} and can be used as alternative designs for the Chlofibric acid synthesis experiment in the Introduction. Figure 3 shows the correlation cell plots (CCPs) of the two FODs, whose HFD matrices are in Figure 1 and Figure 2b. These plots, proposed by Jones & Nachtsheim (2011), display the magnitude of the correlation (in terms of the absolute values) between MEs and 2FIs in screening designs. The color of each cell ranges from white (no correlation) to dark (correlation of 1 or close to 1). As expected, both CCPs in Figures 3a and 3b show that the MEs are orthogonal to the 2FIs. Figure 3a shows that there are 21 fully aliased 2FIs pairs. Figure 3b shows that the correlation among MEs is mild and, unlike Figure 3a, none of the 2FIs are fully aliased with the other 2FIs.

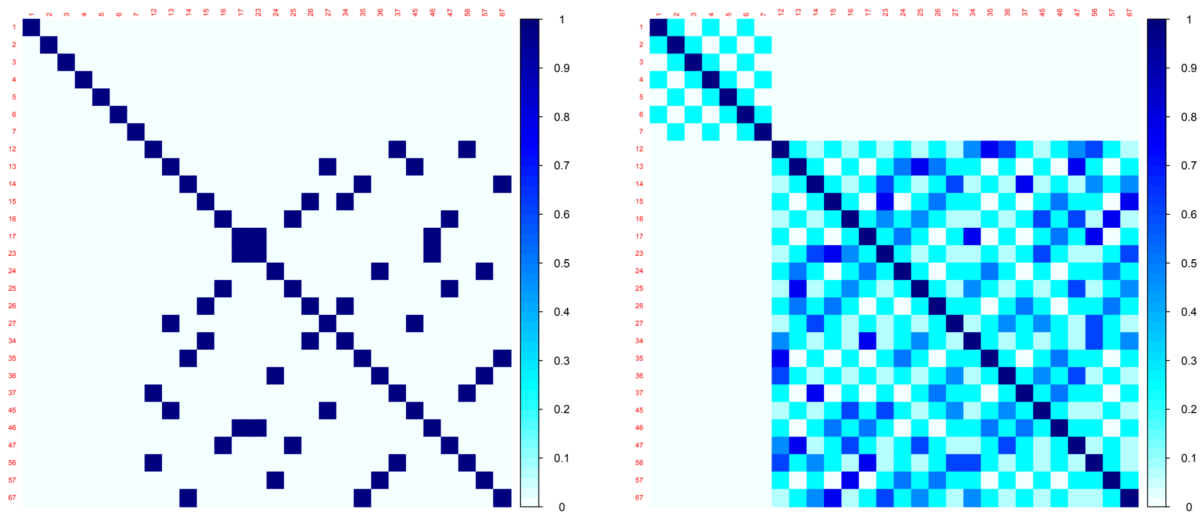
(1)	(2)	(3)	(4)	(5)	(6)	(7)
-1	-1	1	1	1	1	1
1	-1	-1	1	-1	1	-1
1	1	-1	-1	1	-1	-1
-1	1	-1	-1	-1	1	1
-1	1	1	1	-1	-1	-1
-1	-1	1	-1	-1	-1	-1
1	-1	-1	1	-1	-1	1
1	1	1	-1	-1	1	1

(a)

(1)	(2)	(3)	(4)	(5)	(6)	(7)
-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	1	1	-1	1	1	1
-1	1	1	1	-1	1	1
1	-1	1	1	-1	1	-1

(b)

Figure 2: Two HFD matrices of two minimal aliased FODs with the same D_{eff} for $(m,\ n)$ =(7, 8): (a) with $\max_2 = \max_4 = 4$; (b) with $\max_2 = 2$ and $\max_4 = 6$.



(a) (b)

Figure 3: CCPs of the two FODs whose HFD matrices are in Figure 1 and Figure 2b.

We also used $\textbf{FOLD}_1$ with chosen Hadamard matrices of order 12, 16, 20, 24, 28 and 32 to construct strength-3 OAs for 24, 32, 40, 48, 56 and 64 runs, and compare those for 32, 40, 48 runs with the ones of Schoen & Mee (2012) and the regular resolution IV FFDs with $A_3 = A_5 = 0$ for 32 and 64 runs in Table G.3 of Mee (2009). The Hadamard matrices of the order 12, 20, 24 and 28 are the Plackett–Burman designs and the one of the order

32 is `had32.pal.txt` taken from `http://neilsloane.com/hadamard/`. The one order 16 was constructed by $\mathbf{FOLD_2}$. Our constructed strength-3 OAs match those of Schoen & Mee (2012) in terms of A_4, $\max_4$ (and the frequencies of $\max_4$) and df(2FI). For the design with $(m,\ n)$= (10, 16), $\mathbf{FOLD_2}$ produces the solution with $A_4 = 15$ and three counts of $\max_4$=16. The one of Schoen & Mee (2012) has $A_4 = 16.5$ but with a single count of $\max_4$=16.

Irvine, et al. (1996) described a 2^{13-9} experiment investigating the best method to remove lignin during the pulping stage without negatively impacting strength and yield. The 13 factors are: (A) Wood chips presoaked (No or Yes), (B) Chips pre-steamed for 10 min 110^{o}C (No or Yes), (C) Initial effective alkali level (%) 6 or 12, (D) Sulfide level in impregnation (%) 3 or 10; (E) Liquor (Black or White), (F) Liquor/wood ratio (3.5:1 or 6:1), (G) Impregnation temperature (^{o}C) (110 or 150), (H) Impregnation pressure (kPa) (190 or 1140), (J) Impregnation time (min) (10 or 40), (K) Anthraquinone (%) (0.00 or 0.05), (L) Cook temperature (^{o}C) (165 or 170), (M) Water quench (No or Yes), (N) Extended alkali wash for 1 hour (No or Yes). The design generators for this fraction (Figure 4a) are E = -AD, F = -ABCD, G = ABC, H = BCD, J = -AC, K = -BD, L = ACD, M = -AB, and N = -BC. The three response variables are the Kappa number, tear index and yield. This experiment was also described in Mee (2009) p. 184-186.

The data analysis of the experiment in the previous paragraph could only show two marginally significant MEs: H and K. To make the result of this experiment more trustworthy, we assume the scientist repeats it using a fold-over of the mentioned design as the HFD matrix. Let us study four candidate FODs for 13 factors in 32 runs using the HFD matrices in Figures 4a, 4b, 4c and 4d: (a) a 2^{13-8}_{IV} FFD, (b) a strength 3-OA for $(m,\ n)$ = (13, 16) in Table 1, (c) a non-orthogonal FOD for $(m,\ n)$ = (13, 16) with $\max_2$=12 and $\max_4$=10 in Table 2, and (d) a non-orthogonal FOD $(m,\ n)$ = (13, 16) with $\max_2$=4 and $\max_4$=8 in Table 2. It can be seen that the worst correlation of the 2FIs pairs of the first two FODs is 1, of the 3rd FOD is 0.75 (=12/16) and of 4th FOD is 0.5 (=8/16). Figure 5 displays four CCPs whose HFD matrices are in Figure 4. Note that the 2^{13-8}_{IV} FFD (or the one p. 489 of Mee, 2009) and our strength-3 OA for 13 factors in 32 runs (or the one in Table 3 of Schoen & Mee, 2012) both have A_4 =55. For a regular FFD, unlike a strength-3 OA, A_4 is also the number of length 4 words producing full aliasing. As each length-4 word defines three fully aliased 2FIs pairs, this 2_{IV}^{13-8} FFD has 165 (= 3 × 55) fully aliased 2FIs pairs. Our strength-3 OAs only has 30 (= 3 × 10) pairs.

A	B	C	D	E	F	G	H	J	K	L	M	N
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	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	-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	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	-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	-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

(a)

A	B	C	D	E	F	G	H	J	K	L	M	N
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	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	-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	-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	-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	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

(b)

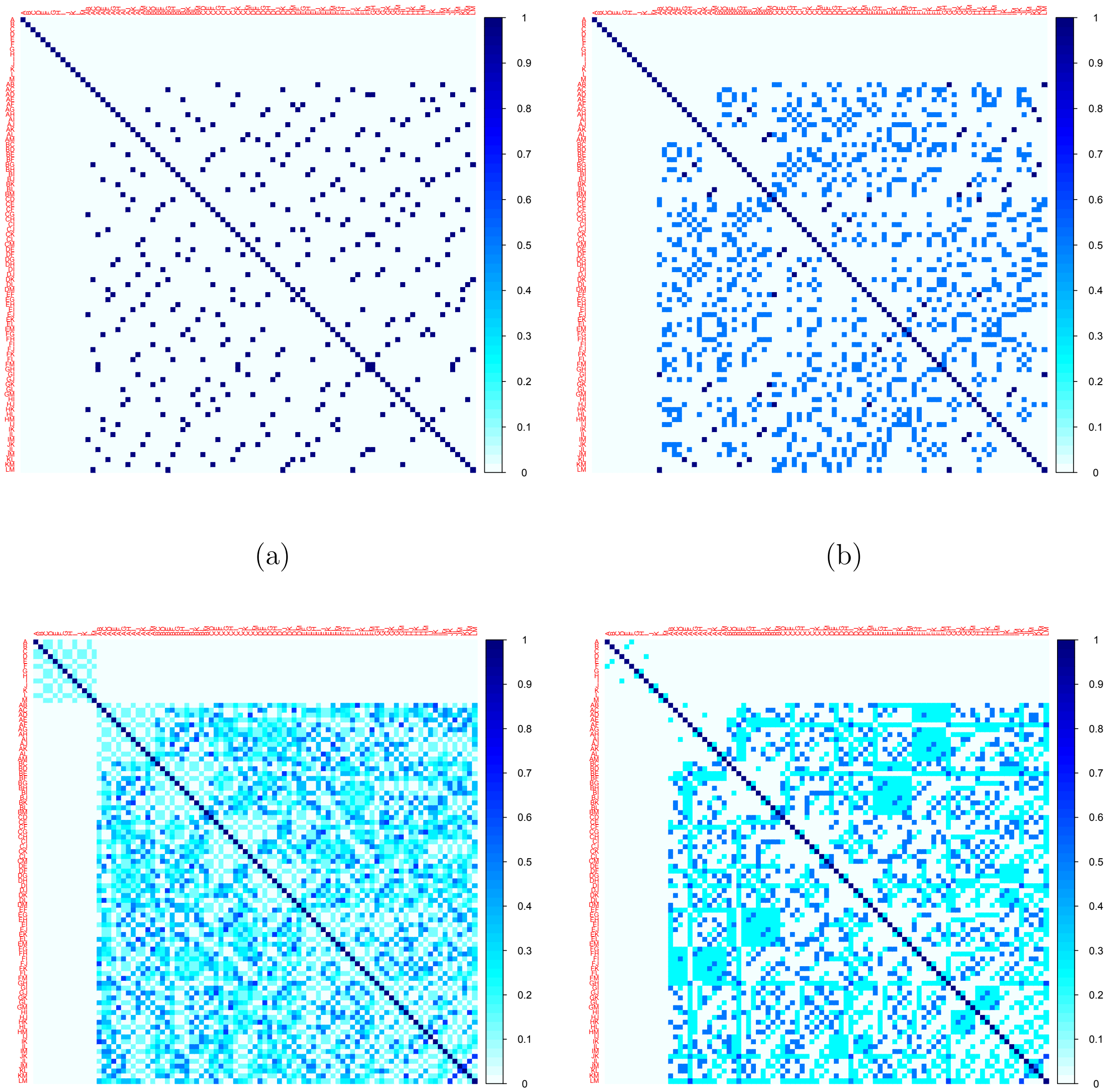
A	B	C	D	E	F	G	H	J	K	L	M	N
1	-1	-1	1	-1	1	1	-1	1	-1	1	-1	-1
-1	-1	1	-1	1	1	1	1	-1	-1	-1	-1	1
1	1	1	1	1	-1	-1	-1	1	1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	1	1	-1	1	1
1	-1	1	-1	-1	-1	-1	1	-1	1	1	1	-1
1	1	-1	-1	1	-1	1	1	1	1	1	-1	1
-1	1	1	1	-1	1	1	-1	-1	1	1	-1	1
1	1	1	-1	-1	1	-1	1	1	-1	1	1	1
-1	1	1	1	-1	-1	1	1	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	-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	-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

(c)

A	B	C	D	E	F	G	H	J	K	L	M	N
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	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	-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	-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	-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	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

(d)

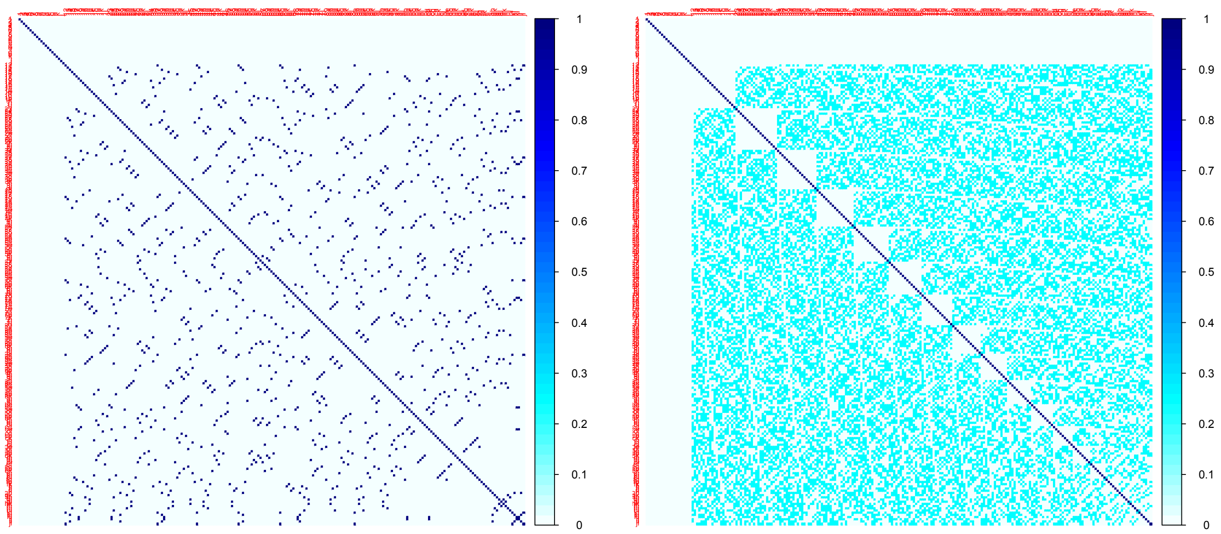
Figure 4: Four HFD matrices of four FODs for $(m,\ n)$ =(13, 16): (a) a 2_{IV}^{13-8} FFD, (b) a strength 3-OA in Table 1, (c) a non-orthogonal FOD with $\max_2$=2 and $\max_4$=10 in Table 2, and (d) a non-orthogonal FOD with $\max_2$=4 $\max_4$=8 in Table 2.



(a) (b) (c) (d)

Figure 5: CCPs of four FODs whose HFD matrices are in Figure 4.

All of our strength-3 OAs match the resolution IV FFDs (with $A_3 = A_5 = 0$) of Mee (2009) for 32 and 64 runs in terms of A_4, except six FFDs for $m = 21$ to 26 in 64 runs. The main difference between these FFDs and ours is that the summations of the type (iv) of the former is either be 0 or 32, while the latter is either 0 and ±8. Thus, all of our strength-3 OA for 64 runs has $\max_4 = 8$, implying the worst correlation among 2FIs is only 0.25 (=8/32). Figure 6 displays two CCPs of two designs for 21 factors in 64 runs: (a) the 2^{21-15}_{IV} FFD on p. 490 of Mee (2009) with $A_4 = 204$ and 612 ($= 3 \times 204$) fully aliased 2FIs pairs (b) our strength-3 OA for the same number of factors and runs. This strength-3 OA has $A_4 = 205$.



(a) (b)

Figure 6: CCPs of two 2-level designs for 21 factors in 64 runs: (a) the FFD of resolution IV of Mee (2009) and (b) our corresponding strength-3 OA.

5 Conclusion

The most popular designs for screening experiments up to this point are still regular FFDs of various resolutions. This is because they are simple to analyze: the MEs are orthogonal to each other, the MEs (and 2FIs) are either orthogonal or fully aliased with other 2FIs. The cost of a regular FFD in a multifactor experiment is a huge number of runs if a resolution V design is used, or a follow-up experiment to disentangle the MEs from 2FIs or 2FIs from other 2FIs. Like the efficient FODs of EJLN, ours offer practitioners additional choices for in terms of the flexible number of design runs. Some FODs expect the practitioners to accept certain mild non-orthogonality among MEs to avoid any 2FI fully aliased.

The HFD matrices of the 49 FODs in Tables 1 and 2, the 115 FODs for 24, 32, 40, 48, 56 and 64 runs and the Java program implementing the FOLD algorithms in Section 3 are in the supplemental material.

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Table 1: Quality measures of some constructed FODs.

m	n	N†	A_2	A_4	$\max_2$	$\max_4$	r_{ave}	r_{max}	D_{eff}	df(2FI)
3	3	6	0.33	0	1 (3)	0 (0)	0.33	0.33	0.877	3
3	4	8	0	0	0 (3)	0 (0)	0	0	1.0	3
4	4	8	0	1	0 (6)	4*(1)	0	0	1.0	3
5	5	10	0.4	1.8	1 (10)	3 (5)	0.2	0.2	0.95	5
5	6	12	0.44	1.22	2 (4)	4 (2)	0.13	0.33	0.933	6
6	6	12	0.67	3.67	2 (6)	4 (6)	0.13	0.33	0.918	6
5	7	14	0.2	1.08	1 (10)	7*(1)	0.14	0.14	0.949	7
6	7	14	0.31	3.24	1 (15)	7*(3)	0.14	0.14	0.92	7
7	7	14	0.43	7.57	1 (21)	7*(7)	0.14	0.14	0.867	7
5	8	16	0	1	0 (10)	8*(1)	0	0	1.0	7
6	8	16	0	3	0 (15)	8*(3)	0	0	1.0	7
7	8	16	0	7	0 (21)	8*(7)	0	0	1.0	7
8	8	16	0	14	0 (28)	8*(14)	0	0	1.0	7
9	9	18	0.74	18.84	5 (1)	9*(7)	0.12	0.56	0.939	9
9	10	20	0.64	16.08	2 (16)	6 (12)	0.09	0.2	0.883	10
10	10	20	0.8	26.8	2 (20)	6 (20)	0.09	0.2	0.852	10
9	11	22	0.3	14.93	1 (36)	5 (42)	0.09	0.09	0.941	11
10	11	22	0.37	24.88	1 (45)	5 (70)	0.09	0.09	0.92	11
11	11	22	0.45	39.09	1 (55)	5 (110)	0.09	0.09	0.88	11
9	12	24	0	14	0 (36)	4 (126)	0	0	1.0	11
10	12	24	0	23.33	0 (45)	4 (210)	0	0	1.0	11
11	12	24	0	36.67	0 (55)	4 (330)	0	0	1.0	11
12	12	24	0	55	0 (66)	4 (495)	0	0	1.0	11
13	13	26	0.46	68.85	1 (78)	11 (13)	0.08	0.08	0.978	13
13	14	28	0.73	61.33	2 (36)	10 (5)	0.07	0.14	0.938	14
14	14	28	0.86	85.86	2 (42)	10 (15)	0.07	0.14	0.936	14
13	15	30	0.35	57.93	1 (78)	15*(10)	0.07	0.07	0.942	15
14	15	30	0.4	81.11	1 (91)	15*(15)	0.07	0.07	0.925	15
15	15	30	0.47	110.6	1 (105)	15*(21)	0.07	0.07	0.893	15
13	16	32	0	55	0 (78)	16*(10)	0	0	1.0	15
14	16	32	0	77	0 (91)	16*(14)	0	0	1.0	15
15	16	32	0	105	0 (105)	16*(21)	0	0	1.0	15
16	16	32	0	140	0 (120)	16*(28)	0	0	1.0	15

†Run size ($= 2n$).

‡Frequencies.

*Designs with fully aliased 2FIs.

Table 2: Constructed FODs with fully alised 2FIs eliminated for $m = 8$ and 16.

m	n	N†	A_2	A_4	$\max_2$	$\max_4$	r_{ave}	r_{max}	D_{eff}	df(2FI)
5	8	16	0.38	0.62	2 (6)	4 (2)	0.15	0.25	0.932	8
6	8	16	0.56	1.88	2 (9)	4 (6)	0.15	0.25	0.913	8
7	8	16	0.75	5.5	2 (12)	6 (3)	0.14	0.25	0.898	8
8	8	16	1	11	2 (16)	6 (8)	0.14	0.25	0.869	8
5	8	16	0.25	0.75	4 (1)	4 (3)	0.05	0.5	0.953	8
6	8	16	0.5	2.5	4 (2)	4 (10)	0.07	0.5	0.921	8
7	8	16	0.75	6	4 (3)	4 (24)	0.07	0.5	0.898	8
8	8	16	1	12	4 (4)	4 (48)	0.07	0.5	0.88	8
13	16	32	0.62	52.38	2 (40)	10 (12)	0.06	0.12	0.95	16
14	16	32	0.75	73.19	2 (48)	10 (17)	0.07	0.12	0.942	16
15	16	32	0.88	99.75	2 (56)	10 (24)	0.07	0.12	0.936	16
16	16	32	1	133	2 (64)	10 (32)	0.07	0.12	0.93	16
13	16	32	0.38	53.5	4 (6)	8 (139)	0.02	0.25	0.973	16
14	16	32	0.44	75.5	4 (7)	8 (197)	0.02	0.25	0.97	16
15	16	32	0.44	102.75	4 (7)	8 (285)	0.02	0.25	0.972	16
16	16	32	0.5	137	4 (8)	8 (380)	0.02	0.25	0.97	16

†Run size ($= 2n$).

‡Frequencies.

§Designs matching the those of EJLN in all quality measures.