A Note on Foldover of 2^{k-p} Designs With Column Permutations

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Abstract

Foldover is a commonly used follow-up strategy in experimental designs. All existing foldover designs were constructed by reversing the sign of columns of the initial design. We propose a new methodology by allowing the permutation of columns in foldover. Focusing on resolution IV designs, we show that almost all designs are better than existing results with respect to the minimum aberration criterion. While augmenting a design by a foldover with column permutations may result in a nonregular combined design, the proposed designs all have a solution of 4.5 or higher, for which no two-factor interaction is fully aliased with any other two-factor interactions.

KEY WORDS: Foldover design; Minimum aberration design; Optimal foldover; Word length pattern.

Two-level fractional factorial designs are among the most commonly used experimental designs. The tradeoff of the run size economy of using such designs is that many effects can be aliased. A commonly used follow-up methodology to break up aliased effects involves adding a second fraction, which is called a *foldover design* (or simply *foldover*), by reversing the signs of one or more columns of the *initial design.* In practice, the strategy usually involves two stages: 1. Run the initial design to identify active main effects and two-factor interactions (2fi's). 2. Use a foldover design to de-alias possible aliased pairs of 2fi's. This strategy has been widely accepted and used in practice. However, there is a major limitation of this approach, which we illustrate below by using a simulated example.

Suppose that an experimenter uses a minimum aberration 2^{6-2}_{IV} design, which is defined by $I = 1235 = 1246 = 3456$, to study six 2-level factors. The responses, as well as the design matrix, are given in Table 1a. The regression results show that all main effects and the two 2fi's, x_1x_5 and x_3x_4, are active. Knowing that each of these 2fi's is aliased with another 2fi, the experimenter decides to use a foldover design to de-alias both pairs by folding over column 5. The responses for the new runs are given in Table 1b, and the analysis of the combined design of those in Tables 1a and 1b identified four active 2fi's: x_1x_5, x_2x_3, x_3x_4, and x_5x_6.

(Table 1 around here.)

The foldover methodology appears to work well for this example, except that there is actually another pair of active 2fi's, x_1x_4 and x_2x_6 that cannot be identified as active effects in the analysis of the initial design. In fact, the true underlying model was given by: $y = 7(x_1+x_2+\cdots+x_6)+5x_1x_5+4x_2x_3+4x_1x_4-4x_2x_6+6x_3x_4+3x_5x_6+\epsilon$, where the error term ϵ follows a normal distribution $N(0, 1)$.

None of the existing foldover strategies is able to de-alias those aliased 2fi pairs in all three words in $I = 1235 = 1246 = 3456$. In the past decade, foldover designs have received surging interest, and most literature focuses on optimal foldover designs. For example, Li and Mee (2002) and Li and Lin (2003) both studied optimal foldovers of regular fractional factorial designs in terms of the resolution and the minimum aberration criteria of the combined design. However, it can be easily seen that the optimal foldover design for $I = 1235 = 1246 = 3456$ can de-alias those aliased 2fi pairs in only two out of three words. For instance, when folding over column 5, the combined design is a resolution-IV design with one length-4 word 1246. This motivates us to extend the traditional foldover strategy by allowing *column permutations*, so as to further increase the resolution of the combined design. Table 1c shows such a design that was obtained by folding over column 5 and permuting columns 5 and 6. The combined design of 1a and 1c has a resolution of 4.5, in which the word 1246 has a length of 4.5 instead of 4, implying that x_1x_2 is only *partially* aliased with x_4x_6. (The fractional length word will be defined in the next section.) For the simulated responses in Table 1c, the stepwise regression method correctly identified all active main effects and the six 2fi's.

The motivation example demonstrates the value of using a foldover design, for which the combined design has a higher resolution than the "optimal" design obtained previously in Li and Lin (2003). This research note answers a simple question: *For a given 2^{k-p} design, can we find a foldover design with respect to the minimum aberration criterion of the combined design by allowing column permutations?* In the reminder of this note, Section 1 discusses the criterion used to select optimal foldover designs with column permutations. In Section 2, we obtain and tabulate a new class of designs. The concluding remarks are given in Section 3.

1 Notations and criterion

Consider a regular fractional factorial 2^{k-p} design $\mathbf{d}$, where k is the number of factors, and p is the number of generators. There are $2^p - 1$ words in its defining relation. Let w_i denote the number of words with length i in the defining relation, then $W(\mathbf{d}) = (w_3, w_4, \ldots, w_k)$ is called the word length pattern (WLP) of the design. The resolution of $\mathbf{d}$ is the smallest r such that $w_r \geq 1$.

In general, a two-level design (which can be either regular or nonregular) is denoted by $\mathbf{d} = [x_{ij}]_{n \times k}$, where $x_{ij} = \pm 1$. Denote the collection of all columns by $D = \{1, \ldots, k\}$. Then for an m-subset of columns $s = \{j_1, \ldots, j_m\} \subseteq D$, Deng and Tang (1999) defined the J-characteristic:

$$J_m(s) = |\sum_{i=1}^{n} x_{ij_1} \cdots x_{ij_m}|. \tag{1}$$

A design $\mathbf{d}$ is regular if $J_m(s) = 0$ or n for all subsets of columns $s \subseteq D$. On the other hand, if there exists an $s \subseteq D$ such that $0 < J_m(s) < n$, then it is a nonregular design. Following Li et al. (2003), we call the term $j_1 \cdots j_m$ a *word* if its J-characteristic defined in (1) does not equal 0. Its *generalized word length* is defined as

$$m + (1 - \frac{1}{n}\sum_{i=1}^{n} x_{ij_1} \cdots x_{ij_m}). \tag{2}$$

Following Li et al. (2003), we define the *extended word length pattern* (EWLP) of $\mathbf{d}$ as

$$(f_1, \cdots, f_{1+(n-1)/n}; f_2, \cdots, f_{2+(n-1)/n} \cdots; f_k, \ldots, f_{k+(n-1)/n}), \tag{3}$$

in which $f_{i+j/n}$ is the number of length-$(i + j/n)$ words. (In the remainder of the note, we shall only display EWLP for $i \geq 4$ because all designs discussed are of resolution IV or higher.)

When a regular design is augmented by its foldover with column permutations, the length of an m-letter word in the combined design equals either m or $m+0.5$. To see this, suppose that defining relations of the initial design $\mathbf{d}$ and its foldover $\mathbf{d}'$ are given respectively by $I(\mathbf{d}) = c_{11} = c_{12} = \cdots = c_{1u}$ and $I(\mathbf{d}') = c_{21} = c_{22} = \ldots = c_{2u}$, where u is the number of words in the defining relation of each design. Then we can obtain two sets: a *partial set* that contains words appearing in either $I(\mathbf{d})$ or $I(\mathbf{d}')$ (but not in both), and a *full set* that contains words appearing in both defining relations. A word in the full set implies full aliasing, and its word length is equal to number of factors in the word. For words in the partial set, their word lengths can be computed by (2). Because the run size of the combined design is twice as large as the one for the initial design, the length of a word in the partial set is equal to the number of factors in the word plus 0.5.

In the illustrative example, the initial design is defined by $I(\mathbf{d}) = 1235 = 1246 = 3456$. The foldover design resulting from foldover on 5 and permutations on 5 and 6 has $I(\mathbf{d}') = -1236 = 1245 = -3456$. Thus, $D_{partial} = \{1235, 1246, -1236, 1245\}$, and $D_{full} = \{\}$. The combined design has EWLP=(0,4;0,0), in which $f_4 = 0$ and $f_{4.5} = 4$. It has 0 length-4 word and 4 length-4.5 words, and its resolution is 4.5.

2 Optimal foldovers with column permutations

We now develop a class of optimal foldover plans with column permutations with respect to the EWLP criterion. For a given 2^{k-p} design $\mathbf{d}$, denote its *foldover plan* γ as the collection of columns whose signs are to be reversed in the foldover design $\mathbf{d}' = \mathbf{d}(\gamma, \delta)$, where δ denotes the permutations of columns $1, \ldots, k$. Then the optimal foldover design is the one such that

$$\text{EWLP}([{}^{\mathbf{d}}_{\mathbf{d}(\gamma^*,\delta^*)}]) = min_{\gamma,\delta}\ \text{EWLP}([{}^{\mathbf{d}}_{\mathbf{d}(\gamma,\delta)}]). \tag{4}$$

Note that for a k-factor design, the number of cases considered in (4) is equal to $2^k \times k!$, which can be substantially large. Li and Lin (2003) proved that, for a regular 2^{k-p} design, all foldover plans are equivalent to a *core foldover plan* that only involves the p generated factors. It can be easily shown that this still holds for foldover with permutations. Thus, the number of computations can be reduced to $2^p \times k!$.

We studied optimal foldover designs with column permutations of a class of 16-run and 32-run resolution-IV designs cataloged in Chen, Sun, and Wu (1993). Their foldovers were studied previously in Montgomery and Runger (1996) and Li and Lin (2003). The results are summarized in Table 2. For $n = 16$ and $n = 32$, $k \leq 9$, we used an exhaustive search method that evaluated all $2^p \times k!$ cases. For $n = 32$ and $k = 10, 11$, the number of cases became prohibitively large. We evaluated a very large number of randomly chosen permutations (by stopping the program after it was run for 168 hours on a 3.40GHz-CPU PC). As there are many permutations that would produce the same foldover designs in terms of the EWLP criterion of the combined design, the results reported in the table for $n = 32$ and $m \geq 10$ are considered to be *very* close to (if not exactly the same) optimal results.

The results in Table 2 are very promising. Among the 21 cases, with the exception of one design (design 7-2.2), *all foldover designs result in a higher resolution when column permutations are implemented.* For design 7-2.2, the optimal foldover without column permutations has a combined design of resolution IV, which cannot be improved further with column permutations. For design 7-2.1, the optimal foldover without column permutations is $\gamma^* = \{6\}$, resulting in a combined design of resolution V. In comparison, by using $\gamma^* = \{6\}$ with columns permutations of $\delta^* = 1234576$ (that involves a swap of columns 6 and 7 of the initial design), the new combined design has the EWLP = (0,0;0,4), which is shown as [0 0][0 4] in Table 2. (For simplicity, with the exception design 7-2.2, we only report the EWLP for words with four and five letters, which is displayed in the form of two brackets.) Thus, the combined design for design 7-2.1 is of resolution 5.5 with four length-5.5 words. In all other 19 cases, the resolution of the combined design is improved from 4 for foldovers without column permutations to 4.5 for the new optimal foldover with column permutations. This improvement from a resolution 4 to 4.5 is substantial, as no 2fi is fully aliased with another 2fi in a resolution-4.5 design.

3 Discussions

In this note we proposed a new class of optimal foldover designs with column permutations, which are shown to have better extended word length patterns than existing optimal foldovers. The trade-off is that the resulting combined designs are generally nonregular designs, which may pose additional challenges to data analysis. Analysis of nonregular designs has been extensively discussed in the literature. See Wu and Hamada (2009) for a review. For more recent discussions, see Mee (2013) and Draguljic et al. (2014).

We note that the proposed approach is related to the earlier work on *equivalent family*, which was proposed by Addelman (1969). Two defining relations are said to be equivalent if one can be obtained from another by interchanging factors in a word. From this perspective, the initial design $\mathbf{d}$ and its foldover with column permutations $\mathbf{d}'$ can be considered from the equivalent family. The idea of combining equivalent family of designs has been explored to construct efficient designs. For example, Pajak and Addelman (1975) developed a criterion for determining the minimum number of blocks of 2^{n-m}_{III} designs such that the combined design could estimate all main effects and 2fi's. More recently, Mee (2004) gave a comprehensive review on the alternatives to the usual orthogonal resolution V designs, in which the combination of designs from the equivalent family was also discussed. Our proposed methodology is distinctive from these studies in two aspects: First, the proposed foldover approach adds only *one* foldover to the initial design, whereas some of previous approaches may require adding *several* blocks. Second, we focus on optimal foldover designs in terms of the EWLP criterion, whereas other criteria were considered in previous studies.

The foldover is just one of the follow-up experiment strategies in the literature. Alternative approaches include the D-optimal augmented design (Mitchell, 1974), the Bayesian approach for augmenting 2^{k-p} designs proposed by Meyer et al. (1996), and semi-foldover design (Mee and Peralta, 2000). For *even* designs, in which their defining relation consists entirely of even-length words, Mee and Xiao (2008) studied optimal foldovers and semi-foldovers for resolution IV designs. We compared our designs with the corresponding D-optimal augmented designs. As an example, consider the 2^{6-2} design in Table 1a. As the analysis of the initial design identified two active 2fi's from two aliasing sets: $x_1x_2x_3x_5$ and $x_3x_4x_5x_6$, we constructed two D-optimal augmented designs in JMP. The first one $\mathbf{d}_1$ is D-optimal in terms of the model consisting of all main effects and the 11 2fi's involved in the two aliasing sets. The second design $\mathbf{d}_2$ is D-optimal in terms of the model consisting of all main effects and all 15 2fi's. The results are encouraging for the proposed foldover designs. First, neither $\mathbf{d}_1$ nor $\mathbf{d}_2$ was level-balanced. In comparison, our design is orthogonal with respect to main effects. Second, we computed the D-criterion values in terms of the true model consisting of the intercept and 12 active effects: $x_1, \ldots, x_6, x_1x_5, x_2x_3, x_1x_4, x_2x_6, x_3x_4, x_5x_6$. The standardized D values for the two combined designs, $\mathbf{d}$ plus $\mathbf{d}_1$ and $\mathbf{d}$ plus $\mathbf{d}_2$, are .9205 and .9365, respectively. In comparison, the combined design of $\mathbf{d}$ and its optimal foldover with column permutations has a D-value of .9567.

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Table 1. A 16-run Design Generated by 5=123 and 6=124

(a) Initial design

Runs	x1	x2	x3	x4	x5	x6	y
1	-1	-1	-1	-1	-1	-1	-26.09
2	1	-1	-1	-1	1	1	16.11
3	-1	1	-1	-1	1	1	0.88
4	1	1	-1	-1	-1	-1	-12.98
5	-1	-1	1	-1	1	-1	-29.93
6	1	-1	1	-1	-1	1	-15.58
7	-1	1	1	-1	-1	1	-0.82
8	1	1	1	-1	1	-1	11.84
9	-1	-1	-1	1	-1	1	-15.77
10	1	-1	-1	1	1	-1	0.16
11	-1	1	-1	1	1	-1	-19.56
12	1	1	-1	1	-1	1	-3.11
13	-1	-1	1	1	1	1	14.98
14	1	-1	1	1	-1	-1	0.60
15	-1	1	1	1	-1	-1	17.20
16	1	1	1	1	1	1	58.10

(b) Optimal foldover design (Foldover on column 5)

Runs	1'=1	2'=2	3'=3	4'=4	5'=-5	6'=6	y
17	-1	-1	-1	-1	1	-1	-26.79
18	1	-1	-1	-1	-1	1	-12.30
19	-1	1	-1	-1	-1	1	-9.12
20	1	1	-1	-1	1	-1	5.58
21	-1	-1	1	-1	-1	-1	-27.65
22	1	-1	1	-1	1	1	12.02
23	-1	1	1	-1	1	1	8.67
24	1	1	1	-1	-1	-1	-4.63
25	-1	-1	-1	1	1	1	-5.55
26	1	-1	-1	1	-1	-1	-17.99
27	-1	1	-1	1	-1	-1	-14.93
28	1	1	-1	1	1	1	28.46
29	-1	-1	1	1	-1	1	5.53
30	1	-1	1	1	1	-1	18.00
31	-1	1	1	1	1	-1	14.41
32	1	1	1	1	-1	1	27.96

(c) Optimal foldover with permutation (Foldover on 5. Permutation of columns 5 and 6)

Runs	1'=1	2'=2	3'=3	4'=4	5'=6	6'=-5	y
17	-1	-1	-1	-1	-1	1	-10.00
18	1	-1	-1	-1	1	-1	-9.88
19	-1	1	-1	-1	1	-1	-11.43
20	1	1	-1	-1	-1	1	-13.61
21	-1	-1	1	-1	-1	-1	-30.58
22	1	-1	1	-1	1	1	14.01
23	-1	1	1	-1	1	1	8.49
24	1	1	1	-1	-1	-1	-3.18
25	-1	-1	-1	1	1	1	-5.33
26	1	-1	-1	1	-1	-1	-18.67
27	-1	1	-1	1	-1	-1	-14.48
28	1	1	-1	1	1	1	27.43
29	-1	-1	1	1	1	-1	-13.83
30	1	-1	1	1	-1	1	16.95
31	-1	1	1	1	-1	1	16.57
32	1	1	1	1	1	-1	44.67

Table 2. Optimal Foldover Plans for Resolution IV Designs With and Without Column Permutations

Runs	*k-p*	Genarating relations	Initial $W(\boldsymbol{d})$	Foldover with permutation Foldover plan (γ)	R	$EWLP(\boldsymbol{D}(\gamma))$
n=16	6-2.1	5=123,6=124	(3 0 0)	γ={5}, perm=123465	4.5	[0 4] [0 0]
				γ={5}	4	[1 0] [0 0]
	7-3.1	5=123,6=124,7=134	(7 0 0 0)	γ={5}, perm=1234675	4.5	[0 12] [0 0]
				γ={5}	4	[3 0] [0 0]
	8-4.1	5=123,6=124,7=134, 8=234	(14 0 0 0)	γ={7,8}, perm=12346758 γ={5,6}	4.5 4	[0 24] [0 0] [6 0] [0 0]
n=32	7-2.1	6=1234,7=1245	(1 2 0 0)	γ={6}, perm=1234576	5.5	[0 0] [0 4]
				γ={6}	5	[0 0] [1 0]
	7-2.2	6=123,7=145	(2 0 1 0)	γ={6,7}, perm=1234567	6	[0 0] [0 0] [1 0]
				γ={6,7}	6	[0 0] [0 0] [1 0]
	7-2.3	6=123,7=124	(3 0 1 0)	γ={6}, perm=1234576	4.5	[0 4] [0 0]
				γ={6}	4	[1 0] [0 0]
	8-3.1	6=123,7=124,8=2345	(3 4 0 0)	γ={6}, perm=12354687	4.5	[0 4] [0 8]
				γ={6}	4	[1 0] [2 0]
	8-3.2	6=123,7=124,8=135	(5 0 2 0)	γ={7,8}, perm=12345876	4.5	[0 6] [0 0]
				γ={7,8}	4	[1 0] [0 0]
	8-3.3	6=123,7=124,8=125	(6 0 0 0)	γ={6,7}, perm=12345687	4.5	[0 8] [0 0]
				γ={6,7}	4	[2 0] [0 0]
	8-3.4	6=123,7=124,8=134	(7 0 0 0)	γ={6}, perm=12345786	4.5	[0 12] [0 0]
				γ={6}	4	[3 0] [0 0]
	9-4.1	6=2345,7=1345,8=1245, 9=1235	(6 8 0 0)	γ={8,9}, perm=123458967 γ={6,7}	4.5 4	[0 8] [0 16] [2 0] [4 0]
	9-4.2	6=123,7=124,8=134, 9=2345	(7 7 0 0)	γ={8,9}, perm=123457869 γ={6,7}	4.5 4	[0 12] [0 12] [3 0] [3 0]
	9-4.3	6=123,7=124,8=135, 9=145	(9 0 6 0)	γ={6,7,8}, perm=123459786 γ={6,7,8}	4.5 4	[0 12] [0 0] [3 0] [0 0]
	9-4.4	6=123,7=124,8=134, 9=125	(10 0 4 0)	γ={7,9}, perm=123547986 γ={8,9}	4.5 4	[0 16] [0 0] [3 0] [0 0]
	9-4.5	6=123,7=124,8=134, 9=234	(14 0 0 0)	γ={8,9}, perm=123457869 γ={6,7}	4.5 4	[0 24] [0 0] [6 0] [0 0]
	10-5.1	6=1234,7=1235,8=1245, 9=1345, 10=2345	(10 16 0 0)	γ={9,10}, perm=12346591078 γ={6,7}	4.5 4	[0 16] [0 32] [4 0] [8 0]
	10-5.2	6=123,7=124,8=135, 9=145, 10=12345	(15 0 15 0)	γ={6}, perm=12345689710 γ={6,7,8}	4.5 4	[0 24] [0 0] [5 0] [0 0]
	10-5.3	6=123,7=124,8=134, 9=125, 10=135	(16 0 12 0)	γ={8,9}, perm=12345786109 γ={8,9}	4.5 4	[0 26] [0 0] [6 0] [0 0]
	10-5.4	6=123,7=124,8=134, 9=234, 10=125	(18 0 8 0)	γ={8,9,10}, perm=12345786910 γ={8,9,10}	4.5 4	[0 30] [0 0] [6 0] [0 0]
	11-6.1	6=123,7=124,8=134, 9=125, 10=135, 11=145	(25 0 27 0)	γ={8,10,11}, perm=1234579106118 γ={6,8,9}	4.5 4	[0 42] [0 0] [10 0] [0 0]
	11-6.2	6=123,7=124,8=134, 9=234, 10=125, 11=135	(26 0 24 0)	γ={6,10}, perm=1234578611109 γ={7,8,10}	4.5 4	[0 46] [0 0] [10 0] [0 0]