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A note on optimal foldover design

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Abstract

This note provides a theoretical justification for the optimal foldover plans for two-level designs, including the regular 2^{s-p}, non-regular, saturated and supersaturated designs.
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Foldover is a classic technique that reverses the signs of one or more factors in the initial design for the follow-up experiment (called a foldover design). This standard strategy can be found in the literature. The conventional wisdom is to reverse signs for all factors. The foldover plan for reversing only one factor was discussed by Box et al. (1978) to de-alias the specific factor from all other factors. Montgomery and Runger (1996) studied foldover for resolution IV designs. Using an exhausted search, Li and Lin (2003) and Li and Mee (2002) recently gave all optimal foldover plans for regular two-level fractional factorial designs, in terms of the aberration criterion of the combined design. Li et al. (2003) studied optimal foldover plans for non-regular two-level factorial designs in terms of the generalized minimum aberration of the combined design. A theoretical justification, however, is lacking. In this note, we will provide a theoretical justification for optimal foldover design, based on uniformity criterion.

Consider a two-level fractional factorial design with n runs and s factors, denoted as $T = (t_1, t_2, \ldots, t_s) = (t_{ij})$, $t_{ij} = \pm 1$. Define a foldover plan as the set of factors whose signs are reversed in the foldover design. This plan is denoted by $\gamma = \delta_1 \cdots \delta_s$, where $\delta_i = 1$ if the ith column

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of T is reversed otherwise 0. The corresponding foldover plan space then is denoted by Γ with 2^s possible foldover plans. For the foldover plan γ, let $m = \sum_{i=1}^{s} \delta_i$. When $m = s$, the foldover plan is called a full foldover plan in the statistical literature. Specifically, for a two-level factorial design T with design columns, t_i's, and a given foldover plan γ, a new $2n$-run and s-factor combined design $T(\gamma)$ is then

$$T(\gamma) = \begin{pmatrix} t_1 & t_2 & \cdots & t_s \\ (-1)^{\delta_1} t_1 & (-1)^{\delta_2} t_2 & \cdots & (-1)^{\delta_s} t_s \end{pmatrix}.$$

Uniformity has received a great deal of attention in the recent design literature (see, for example, Fang and Mukerjee, 2000; Fang and Lin, 2003). There are many measures of uniformity. Among them, the centered L_2-discrepancy (CD for short) has good properties (Hickernell, 1998a). The squared CD can be expressed in the close form

$$(\text{CD}(\mathscr{P}))^2 = \left(\frac{13}{12}\right)^s - \frac{1}{n} \sum_{k=1}^{n} \prod_{i=1}^{s} \left(1 - \frac{1}{2}\left|x_{ki} - \frac{1}{2}\right| - \frac{1}{2}\left|x_{ki} - \frac{1}{2}\right|^2\right)$$
$$+ \frac{1}{n^2} \sum_{k=1}^{n} \sum_{j=1}^{n} \prod_{i=1}^{s} \left(1 + \frac{1}{2}\left|x_{ki} - \frac{1}{2}\right| + \frac{1}{2}\left|x_{ji} - \frac{1}{2}\right| - \frac{1}{2}|x_{ki} - x_{ji}|\right),$$

where $\mathscr{P} = \{x_1, \ldots, x_n\}$ is a set of n points on $[0,1)^s$.

For the combined design $T(\gamma) = (t_{ij}^*)$ we can make the transformation from $T(\gamma)$ to a set of $2n$ points on $[0,1)^s$, $\mathscr{P}_{T(\gamma)} = \{x_1, \ldots, x_{2n}\}$, where $x_{ij} = (t_{ij}^* + 2)/4 \in [0,1)$. Then, the CD value of $T(\gamma)$, denoted by $\text{CD}(T(\gamma))$, can be calculated as follows:

$$(\text{CD}(T(\gamma)))^2 = c + \frac{1}{2n^2} \sum_{k=1}^{n} \sum_{j=1}^{n} \prod_{i=1}^{s} \left(\frac{5}{2} - \frac{1}{2}|x_{ki} - x_{ji}| - \frac{1}{2}|x_{ki} + (-1)^{\delta_i+1} x_{ji} - \delta_i|\right), \qquad (1)$$

where $c = (13/12)^s - 2(35/32)^s$. From (1), it is clear that the value $\text{CD}(T(\gamma))$ mainly concerns the first n points of $\mathscr{P}_{T(\gamma)}$ and the foldover plan γ. For an initial design T, different CD-values of $T(\gamma)$ are given by different foldover plans γ.

For regular two-level designs, Fang and Mukerjee (2000) obtained a link between CD and the word length pattern, that can be extended to non-regular two-level designs (see Eqs. (A.1) and (A.2) in Appendix A). We can see the minimum (generalized) aberration criterion and the uniformity criterion in the sense of the CD are *almost* equivalent for two-level factorials. We have checked all designs given in Chen et al. (1993) and found that these two criteria are consistent without any exception. We thus define such an "almost equivalent" as "*A-equivalent*". Thenceforward, the *optimal foldover plan* in this paper is defined as the foldover plan γ such that its combined design T_γ has the smallest CD-value over Γ. The main advantages of the uniformity criterion are: (1) it is applicable to regular and non-regular two-level designs and (2) it is very easy to compute.

For convenience in this paper, an $E(s^2)$-optimal supersaturated design means that the Hamming distance (see MacWilliams and Sloane, 1977) of any two distinct rows of the design is a constant (see Nguyen, 1996; Tang and Wu, 1997). Following Mukerjee and Wu (1995), the Hamming distance

of any two distinct rows of a saturated orthogonal array is also a constant. We have the following theorem whose proof is given in Appendix A.

Theorem 1. (i) *For regular 2^{s-p} designs, the optimal foldover plan given here is* A-*equivalent to an optimal foldover plan proposed by Li and Lin (2003).*

(ii) *For non-regular two-level factorial designs, the optimal foldover plan given here is* A-*equivalent to an optimal foldover plan proposed by Li et al. (2003).*

(iii) *If the initial design is a two-level saturated orthogonal array or an $E(s^2)$-optimal supersaturated two-level design, then the optimal foldover plan is the full foldover plan.*

(iv) *For fixed m and the initial design being a two-level saturated orthogonal array or an $E(s^2)$-optimal supersaturated two-level design, the optimal foldover plan γ^* is* A-*equivalent to the one γ such that N_γ has the minimum generalized aberration, where N_γ is the sub-design of T consisting of s–m unchanged columns under γ.*

(v) *Under the full foldover plan, all initial designs with identical even-length words result in the identical* CD-*value for the combined design.*

Remark 1. Note that similar conclusions also hold if the wrap-around L_2-discrepancy or the symmetric L_2-discrepancy, proposed by Hickernell (1998a, b) and discussed by Fang and Ma (2001), serves as a measure of uniformity.

Remark 2. The statement (v) indicates that if the initial design is a uniform design with even resolution, then the resulting combined design under the full foldover plan has the lowest discrepancy. This fact does not hold for initial designs of odd resolution. For example, consider two regular designs, D_1 and D_2, both with 16 runs and seven factors. Suppose that the generating relations of D_1 and D_2 are $5 = 12$, $6 = 13$, $7 = 234$, and $5 = 12$, $6 = 13$, $7 = 23$, with word length patterns $(0, 0, 2, 3, 2, 0, 0)$ and $(0, 0, 4, 3, 0, 0)$, respectively. It is clear that both designs have resolution III and the CD-value of D_1 is less than that of D_2. However, the resulting combined designs under full foldover plan have the same generalized word length pattern $(0, 0, 0, 3, 0, 0, 0)$ and same CD-value 0.287896.

Remark 3. It is important to note from (v) that, under the full foldover plan, different initial designs may result in the same CD-value for the combined designs. Consider, for example, two 16-run, 5-factor designs with generating relations $5 = 1234$ and $5 = 12$. One design is of resolution V, and the other one is of resolution III. However, both of their combined designs under the full foldover plan are full factorial designs.

Acknowledgements

Appendix A. Proof of Theorem 1

Fang and Mukerjee (2000) provided the following analytic connection between uniformity and aberration in regular two-level designs:

$$(\mathrm{CD}(T(\gamma)))^2 = c + \left(\frac{9}{8}\right)^s \left[1 + \sum_{i=1}^{s} \frac{A_i(T(\gamma))}{9^i}\right], \tag{A.1}$$

where c is defined in (1) and $(A_1(T(\gamma)), \ldots, A_s(T(\gamma)))$ is the word length pattern of design $T(\gamma)$. From (A.1), it is clear that the minimum aberration criterion and the uniformity criterion in the sense of the CD are A-equivalent for regular 2^{s-p} factorials. Recall that the optimal foldover plan γ^* proposed by Li and Lin (2003) is the one such that $T(\gamma)$ has minimum aberration. Thus, statement (i) follows.

For non-regular two-level designs, Ma and Fang (2001) proved the following formula:

$$(\mathrm{CD}(T(\gamma)))^2 = c + \left(\frac{9}{8}\right)^s \left[1 + \sum_{i=1}^{s} \frac{A_i^{\mathrm{g}}(T(\gamma))}{9^i}\right], \tag{A.2}$$

where c is defined in (1) and $(A_1^{\mathrm{g}}(T(\gamma)), \ldots, A_s^{\mathrm{g}}(T(\gamma)))$ is the generalized word length pattern of $T(\gamma)$ (proposed by Ma and Fang, 2001; Xu and Wu, 2001). It is well known that the criterion of minimum generalized aberration, independently proposed by Ma and Fang (2001) and Xu and Wu (2001) is essentially identical for two-level designs. From (A.2) we can see the CD and the generalized minimum aberration are A-equivalent for non-regular two-level factorials. Note that the optimal foldover plans proposed by Li et al. (2003) are in terms of the generalized minimum aberration. Therefore, statement (ii) is proved.

Let $\mathrm{DHT}(x_k, x_j)$ and $\mathrm{DHN}(x_k, x_j)$ be the Hamming distance between the kth and jth rows in T and N_γ, respectively. The identity (1) can be expressed in terms of Hamming distances as follows:

$$(\mathrm{CD}(T(\gamma)))^2 = c + \frac{1}{2n^2} \sum_{k=1}^{n} \sum_{j=1}^{n} \left[\left(\frac{5}{4}\right)^{s-\mathrm{DHT}(x_k, x_j)} + \left(\frac{5}{4}\right)^{s-m+\mathrm{DHT}(x_k, x_j)-2\mathrm{DHN}(x_k, x_j)}\right]. \tag{A.3}$$

When $\mathrm{DHT}(x_k, x_j) = \lambda$ for all pairs (k, j) $(k \neq j)$, (A.3) becomes

$$(\mathrm{CD}(T(\gamma)))^2 = c + \frac{1}{2n} \left[\left(\frac{5}{4}\right)^s + (n-1)\left(\frac{5}{4}\right)^{s-\lambda} + \left(\frac{5}{4}\right)^{s-m} - \left(\frac{5}{4}\right)^{s-m+\lambda}\right]$$

$$+ \frac{1}{2n}\left(\frac{5}{4}\right)^{s-m+\lambda} \sum_{j=0}^{s-m} E_j(N_\gamma)\left(\frac{16}{25}\right)^j, \tag{A.4}$$

where $(E_0(T), E_1(T), \ldots, E_s(T))$ is the distance distribution of T (see Ma and Fang, 2001).

Now, it is not hard to see that $(\mathrm{CD}(T(\gamma)))^2$ achieves its minimum value if and only if $m = s$, which establishes statement (iii).

From (A.4) and two formulae:

$$E_j(N_\gamma) = \frac{n}{2^{s-m}} \sum_{i=0}^{s-m} P_j(i; s-m) A_i^{\mathrm{g}}(N_\gamma)$$

and

$$\sum_{j=0}^{s-m} P_j(i; s-m) a^j = (1+a)^{s-m-i}(1-a)^i,$$

where

$$P_j(i; t) = \sum_{r=0}^{j} (-1)^r \binom{i}{r} \binom{t-i}{j-r}$$

is the Krawtchouk polynomial (see MacWilliams and Sloane, 1977), we have

$$(\mathrm{CD}(T(\gamma)))^2 = c + \frac{1}{2n} \left[\left(\frac{5}{4}\right)^s + (n-1)\left(\frac{5}{4}\right)^{s-\lambda} + \left(\frac{5}{4}\right)^{s-m} - \left(\frac{5}{4}\right)^{s-m+\lambda} \right]$$

$$+ \frac{1}{2} \left(\frac{5}{4}\right)^\lambda \left(\frac{41}{40}\right)^{s-m} \left[1 + \sum_{t=1}^{s-m} \left(\frac{9}{41}\right)^t A_t^{\mathrm{g}}(N_\gamma) \right]. \tag{A.5}$$

From (A.5), it is clear that, for fixed m, $(\mathrm{CD}(T(\gamma)))^2$ achieves its minimum value is A-equivalent to that N_γ has minimum generalized aberration. Hence, statement (iv) follows.

When $m = s$, (A.3) becomes

$$(\mathrm{CD}(T(\gamma)))^2 = c + \frac{1}{2n} \sum_{i=0}^{s} E_i(T) \left[\left(\frac{5}{4}\right)^{s-i} + \left(\frac{5}{4}\right)^i \right]$$

$$= c + \left(\frac{9}{8}\right)^s + \frac{1}{2} \left(\frac{9}{8}\right)^s \sum_{i=1}^{s} [1 + (-1)^i] \frac{A_i^{\mathrm{g}}(T)}{9^i}. \tag{A.6}$$

It is clear that $(\mathrm{CD}(T(\gamma)))^2$ depends only on even-length words of T. Statement (v) is proved. $\quad\square$

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