



# An efficient methodology for constructing optimal foldover designs in terms of mixture discrepancy



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## ABSTRACT

Mixture discrepancy criterion (Zhou et al., 2013) is more reasonable than other discrepancies criteria for measuring the uniformity of experimental designs. In this paper, we take the mixture discrepancy criterion as the optimality measure to assess optimal foldover plans, which serve as benchmarks for constructing optimal foldover and combined designs (see Definition 2). New analytical expressions as well as new lower bounds of the mixture discrepancy criterion for both symmetric two-level and three-level combined designs under general foldover plans are obtained. We also describe necessary conditions for the existence of optimal combined designs meeting these lower bounds. An algorithm for searching the optimal foldover plans is also developed. Illustrative examples are provided, where numerical studies lend further support to our theoretical results. These results may help to provide some powerful and efficient algorithms for searching the optimal foldover and combined designs.

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## 1. Introduction

Practitioners often use multilevel factorial designs to investigate the effects of several factors simultaneously. For any factorial design with  $s$ -level and  $m$  factors, the number of runs  $n$  required by a full  $s^m$  factorial design increases geometrically as the number of factors  $m$  and/or the number of levels  $s$  increases. This makes it more desirable to use fractional factorial designs to reduce the number of runs. One consequence of using fractional factorial designs is the aliasing of factorial effects.

A standard follow-up strategy discussed in many textbooks involves adding a second fraction, called a foldover design. Foldover of a fractional factorial design is a quick technique to create a design with twice as many runs, which typically releases aliased factors or interactions. A standard approach to foldover two-level fractional factorial designs is to reverse the plus and minus signs of one or more columns of the original design. Many works on optimal foldover plans for two-level designs in terms of aberration criterion or clear effects criterion have been published. The reader can refer to Li and Lin (2003); Li, Lin, and Ye (2003); Li, Liu, and Zhang (2005), Montgomery and Runger (1996) and Wang, Robert, and John (2010).

In the last few years, much attention has been paid in employing the discrepancy criterion to assess the optimal foldover plans. The foldover plan such that the combined design (original design plus its corresponding foldover design) has the smallest discrepancy value over all foldover plans is called the optimal foldover plan. Fang, Lin, and Qin (2003) initiated the use of uniformity criterion measured by centered  $L_2$ -discrepancy criterion to obtain the optimal foldover plan. Lei, Qin,

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and Zou (2010); Lei, Ou, Qin, and Zou (2012) obtained some lower bounds of centered  $L_2$ -discrepancy criterion of combined designs when all Hamming distances between any distinct pair of runs of the two-level initial design are equal. Subsequently, Ou, Chatterjee, and Qin (2011) obtained some lower bounds of various discrepancies criteria of combined designs for general case. Qin, Chatterjee, and Ou (2013) further extended the ones of Ou et al. (2011) for symmetric designs to a set of asymmetric designs under a special case. Ou, Qin, and Cai (2014, 2015) obtained the optimal foldover plans of mixed two- and three-level designs and three-level designs with minimum wrap-around  $L_2$ -discrepancy criterion, respectively. Recently, Elsayah and Qin (2015a) studied the issue of the optimal foldover plans for three-level designs in view of the uniformity criterion measured by the Lee discrepancy criterion. Finally, Elsayah and Qin (2015c, in press) obtained a new look for optimal foldover two-level and three-level designs in terms of uniformity criteria measured by the commonly used discrepancies criteria in the literature with a comparison study, respectively.

Recently, Zhou, Fang, and Ning (2013) pointed out some unreasonable phenomena associated with the commonly used discrepancies criteria in the literature such as the centered  $L_2$ -discrepancy criterion and the wrap-around  $L_2$ -discrepancy criterion. They proposed a new measurement known as the mixture discrepancy criterion. They proposed that mixture discrepancy criterion satisfies 7 criteria for assessing measures of uniformity introduced in Fang, Li, and Sudjianto (2006). Furthermore Zhou et al. (2013) pointed out some limitations of centered  $L_2$ -discrepancy criterion and the wrap-around  $L_2$ -discrepancy criterion through examples. That is, centered  $L_2$ -discrepancy criterion covers the points near the center insufficiently and this measurement will cause some problems when data is high dimensional, the wrap-around  $L_2$ -discrepancy criterion is not sensitive for each level shift in a certain sense. These limitations may lead to some unreasonable results. The mixture discrepancy criterion performs well under these situations, compared to the centered  $L_2$ -discrepancy criterion and the wrap-around  $L_2$ -discrepancy criterion. Meanwhile, this new discrepancy criterion has a clear geometric meaning and a simple computational formula. This new discrepancy criterion has many good properties and can avoid weaknesses of the centered  $L_2$ -discrepancy criterion and the wrap-around  $L_2$ -discrepancy criterion.

In this paper, we take the mixture discrepancy criterion as the optimality measure to assess the optimal foldover plans and take symmetric factorials with two-level and three-level balanced designs as original designs. A symmetric  $s$ -level balanced design  $\mathcal{D}(n; s^m)$  belonging to a class  $\mathcal{B}(n; s^m)$  corresponds to an  $n \times m$  matrix  $X = (x_1, \dots, x_m)$  such that each column  $x_i$  takes values from a set of  $s$  integers, say  $0, 1, \dots, s-1$ , equally often. By mapping  $f: y \rightarrow (2y+1)/(2s)$ ,  $y = 0, 1, \dots, s-1$ , the  $n$  runs are transformed into  $n$  points in  $\Omega^m = [0, 1]^m$ . The design  $\mathcal{D}$  is also regarded as a set of  $m$  columns  $\mathcal{D} = (x^1, x^2, \dots, x^m)$ , where  $x^j = (x_{1j}, \dots, x_{nj})'$  is the  $j$ th column of  $\mathcal{D}$  and  $j = 1, \dots, m$ . For any symmetric  $s$ -level balanced design  $\mathcal{D} \in \mathcal{B}(n; s^m)$ , its mixture discrepancy criterion value, denoted as  $MD(\mathcal{D})$ , can be expressed in the following closed form

$$[MD(\mathcal{D})]^2 = \left(\frac{19}{12}\right)^m - \frac{2}{n} \sum_{i=1}^n \prod_{k=1}^m \Delta_{ik} + \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \prod_{k=1}^m \nabla_{ijk}, \quad (1.1)$$

where  $\nabla_{ijk} = \frac{15}{8} - \frac{1}{4}|z_{ik} - \frac{1}{2}| - \frac{1}{4}|z_{jk} - \frac{1}{2}| - \frac{3}{4}|z_{ik} - z_{jk}| + \frac{1}{2}|z_{ik} - z_{jk}|^2$ ,  $\Delta_{ik} = \frac{5}{3} - \frac{1}{4}|z_{ik} - \frac{1}{2}| - \frac{1}{4}|z_{ik} - \frac{1}{2}|^2$ ,  $z_{ik} = (2x_{ik} + 1)/2s$ ,  $x_{ik} \in \{0, 1, \dots, s-1\}$ ,  $i = 1, \dots, n$ ,  $j = 1, \dots, n$  and  $k = 1, \dots, m$ .

This paper is organized as follows. Section 2 describes a general structure of multilevel foldover plans based on the mixture discrepancy criterion. In Section 3, new formulations and new lower bounds of the mixture discrepancy for two-level combined designs are obtained. In Section 4, new formulations and new lower bounds of the mixture discrepancy for three-level combined designs are given. An algorithm for searching the optimal foldover plans is also developed in Section 5. In Section 6, illustrative examples are provided, where numerical studies lend further support to our theoretical results. Finally the conclusions and future work are presented in Section 7.

## 2. Optimal foldover plans based on mixture discrepancy

Reversing plus and minus signs of one or more factors is the traditional method to foldover two-level fractional factorial designs. While the method of reversing signs loses its efficacy when factors in the original design have more than two-levels, our method here is good for general  $s$ -level fractional factorial designs.

**Foldover plans.** Define  $\Gamma = \{(\gamma_1, \dots, \gamma_m) | \gamma_j = 0, 1, 2, \dots, s-1; 1 \leq j \leq m\}$ , then for any  $\gamma = (\gamma_1, \dots, \gamma_m) \in \Gamma$ , it defines a foldover plan for any  $s$ -level balanced design  $\mathcal{D} \in \mathcal{B}(n; s^m)$ .

**Foldover designs.** For any design  $\mathcal{D} \in \mathcal{B}(n; s^m)$  and any foldover plan  $\gamma \in \Gamma$ , the foldover design, denoted by  $\mathcal{D}_f$ , is regarded as a set of  $m$  columns  $\mathcal{D}_f = (f^1, f^2, \dots, f^m)$ , where  $f^j = (f_{1j}, \dots, f_{nj})' = (x_{1j} + \gamma_j, \dots, x_{nj} + \gamma_j)' \pmod{s}$  is the  $j$ th column of the foldover design  $\mathcal{D}_f$  and  $j = 1, \dots, m$ . Thus, it is to be noted that each foldover design is generated by a foldover plan.

**Combined designs.** The full design obtained by augmenting the runs of the foldover design  $\mathcal{D}_f$  to those of the original design  $\mathcal{D}$  is called as combined design, denoted by  $\mathcal{D}_c$ , that is,  $\mathcal{D}_c = (\mathcal{D}' \mathcal{D}_f)'$ . Denoted by  $\mathcal{C}(n; s^m)$  the set of all  $s$ -level combined designs.

Under any foldover plan  $\gamma = (\gamma_1, \dots, \gamma_m) \in \Gamma$ , the mixture discrepancy criterion value of the combined design  $\mathcal{D}_c$ , denoted by  $MD(\mathcal{D}_c)$ , can be calculated by the following formula.

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