Fold Over Plan for Uniform Design

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Abstract. This article discusses the fold over problem for uniform design in terms of the centered $L_2$ discrepancy. Both full fold over plan and partial fold over plan are studied. Illustrative examples are given.

Introduction

Uniform design proposed by Fang and Wang in 1980s ([3, 7]) now has been widely used in various fields, such as industry, system engineering and computer designs for its flexible run size and robustness under unknown models. Oftenly, one needs to choose a small size uniform design at the beginning due to, for example a limit of budget, and later to conduct a follow up experiments. How to choose the best follow up experiments for uniform designs to keep the combined design having nice desirable property?

Fold over is a conventional technique that reverses the signs of one or more factors in the initial design for the follow-up experiment. The main benefit of fold over is to de-alias confounding main effects and 2f's in $2^{k-p}$ fractional factorial designs, see Li and Lin(2003)[5] and Li et al. (2003)[6]. Along the same line, Ai, Hickernell and Lin (2008)[1] studied the optimal fold over plans for regular s-level fractional factorial designs by adding another ($s-1$) times of initial runs, where $s$ is any prime or prime power.

A symmetric design is that if for any row(run) $d$, -$d$ is also one of the rows in the design(Ye et al. 2000[8]). In other words, if $d_i$ is a design point, then there exist another point $d_j$ in the design that is the reaction of $d_i$ through the center. A good property of symmetric design is that the estimates of quadratic effects and bilinear interaction effects are uncorrelated with the estimates of linear effects when a polynomial model is used. Note that some uniform designs have such symmetric property, we call them symmetric uniform designs. See Table 1, for example, symmetric uniform designs of 9 runs with different number of 3-level factors, the 5th point is the center point, the (10-$i$)th run is the reaction point of the ith run, as shown in Table 1. Unfortunately, most uniform designs do not have such a symmetric property.

Consider the fold over plan for UDs by inversing the signs of all factors. Denote the different levels of each factor as -(2k+1),...,-3,-1,1,3,...,2k+1 or -k,...,-1,0,1,..., k, then the combined design of the initial and fold over design is a symmetric design. According to the property of centered $L_2$ discrepancy, the fold over design has the same discrepancy as the initial design, if the initial design is a uniform design, then the fold over design is also a uniform design. It is useful when a two-stage experiment to conduct because we have the best design for each stage.

This paper proposed a new method of fold over plan for uniform designs based on the centered $L_2$ discrepancy. It is an extension of fold over plan for 2-level designs, but different from the permutation method usually discussed in existing literature. The propose method has at least 3 virtues as follows. Firstly, doing full fold over plan on uniform design can produce symmetric design and its discrepancy is not bad; Secondly, it is easy to compute, for design of any number of factors and what lever they are,
the optimal fold over plan is easy to get, while the permutation method is difficult to calculate for big number of factors and high levels. Thirdly, as mentioned before, each stage is a uniform design.

Section 2 introduces the properties of full fold over plan for Uds, Sections 3 discusses partial fold over for UDs to keep the combined design uniform, illustrative examples are also provide. Section 4 gives the conclusion and suggests some future work.

| No. | SUD_4(3^2) | SUD_4(3^3) | SUD_4(3^4) |
|-----|-------------|-------------|-------------|
| 1   | 1           | 1           | 1           |
| 2   | 1           | 0           | -1          |
| 3   | -1          | 0           | 1           |
| 4   | 0           | 1           | 0           |
| 5   | 0           | 0           | 0           |
| 6   | 0           | -1          | 1           |
| 7   | -1          | 1           | 0           |
| 8   | -1          | 0           | 1           |
| 9   | -1          | -1          | -1          |
| CD  | 0.019976    | 0.033034    | 0.049364    |

Full Foldover Plan for Uniform Design

Consider the symmetric structure. For any design X, a fold over structure design is U = \( \begin{pmatrix} X \\ X^* \end{pmatrix} \), where \( X^* \) is a full fold over of \( X \). Furthermore let \( X = (x_{ij})_{n \times r} \), \( 0 < x_{ij} < 1 \). Then the center point is \( (\frac{1}{2}, \frac{1}{2}, \ldots, \frac{1}{2}) \) and the reaction point of \( x_{ij} \) is \( x^*_{ij} = 1 - x_{ij} \). The centered \( L_2 \) discrepancy (Hickernell (1998) [4]) of \( X \) denoted as CD(X) is:

| No. | Full fold-over plan | Optimal fold over plan |
|-----|---------------------|------------------------|
| 1   | 1 8 7 6 4 3 4       | 1 8 7 6 4 3 4          |
| 2   | 2 3 5 1 1 6 5       | 2 3 5 1 1 6 5          |
| 3   | 3 4 3 8 8 7 3       | 3 4 3 8 8 7 3          |
| 4   | 4 6 2 2 7 2 7       | 4 6 2 2 7 2 7          |
| 5   | 5 2 8 3 6 4 1       | 5 2 8 3 6 4 1          |
| 6   | 6 1 4 7 3 1 6       | 6 1 4 7 3 1 6          |
| 7   | 7 7 1 4 2 5 2       | 7 7 1 4 2 5 2          |
| 8   | 8 5 6 5 5 8 8       | 8 5 6 5 5 8 8          |
| 9   | 9 1 4 3 4 1 1       | 1 5 3 4 5 1 1          |
| 10  | 10 2 2 8 5 7 4 7    | 2 7 8 5 2 4 7          |
| 11  | 11 3 8 5 2 6 8 3    | 3 1 5 2 3 8 3          |
| 12  | 12 4 7 1 6 3 5 8    | 4 2 1 6 6 5 8          |
| 13  | 13 5 3 7 7 2 7 2    | 5 6 7 7 7 7 2          |
| 14  | 14 6 5 6 1 1 2 6    | 6 4 6 1 8 2 6          |
| 15  | 15 7 6 4 8 3 8 3 4 8 3 3 4 8 3 4 |
| 16  | 16 8 1 2 3 5 6 5    | 8 8 2 3 4 6 5          |
| CD  | 0.06200147          | 0.06138146             |

| No. | Full fold-over plan | Optimal fold over plan |
|-----|---------------------|------------------------|
| 1   | 1 4 3 4 1 1         | 1 5 3 4 5 1 1          |
| 2   | 2 2 8 5 7 4 7       | 2 7 8 5 2 4 7          |
| 3   | 3 8 5 2 6 8 3       | 3 1 5 2 3 8 3          |
| 4   | 4 7 1 6 3 5 8       | 4 2 1 6 6 5 8          |
| 5   | 5 3 7 7 2 7 2       | 5 6 7 7 7 7 2          |
| 6   | 6 5 6 1 1 2 6       | 6 4 6 1 8 2 6          |
| 7   | 7 6 4 8 3 8 3       | 7 3 4 8 1 3 4          |
| 8   | 8 1 2 3 5 6 5       | 8 8 2 3 4 6 5          |
| CD  | 0.06200147          | 0.06138146             |

Table 1. Symmetric uniform designs.

| No. | Full fold-over plan | Optimal fold over plan |
|-----|---------------------|------------------------|
| 1   | (1,1,1,1,1,1,1,1)   | (1,0,1,0,1,0,1,1)      |
| CD  | 0.019976            | 0.033034               |

Table 2. Fold over plan for U8 (8; 87).
\[
[CD(X)]^2 = \left(\frac{13}{12}\right)^2 - 2 \frac{n}{\sum_{k=1}^{n} \prod_{j=1}^{r} \left( 1 + \frac{1}{2} x_{ij} - \frac{1}{2} x_{kj} - \frac{1}{2} x_{li} \right)}
+ \frac{1}{n^2} \sum_{k=1}^{n} \sum_{j=1}^{r} \prod_{i=1}^{s} \left[ 1 + \frac{1}{2} x_{ij} - \frac{1}{2} x_{kj} + \frac{1}{2} x_{li} - \frac{1}{2} x_{ki} - x_{ji} \right].
\]

(1)

Then the centered L2 discrepancy of the combined design U found to be
\[
[CD(U)]^2 = [CD(X)]^2 - \frac{1}{2n^2} \sum_{k=1}^{n} \sum_{j=1}^{r} \prod_{i=1}^{s} \left[ 1 + \frac{1}{2} x_{ij} - \frac{1}{2} x_{kj} + \frac{1}{2} x_{li} - \frac{1}{2} x_{ki} - x_{ji} \right]
+ \frac{1}{2n^2} \sum_{k=1}^{n} \sum_{j=1}^{r} \prod_{i=1}^{s} \left[ 1 + \frac{1}{2} x_{ij} - \frac{1}{2} x_{kj} + \frac{1}{2} x_{li} - \frac{1}{2} x_{ki} - x_{ji} \right].
\]

(2)

Specifically for the 3-level case, when \( X \in U \left( n; 3^r \right), U \left( n; 3^r \right) \) is a set of all 3-level U-type designs, U-type design means three levels appear equally often for every factor, we have the following corollary.

**Corollary 1** For any 3 level U-type design \( X \in U \left( n; 3^r \right) \), define \( h_{ij} = \# \{ k : x_{ik} = x_{jk} \neq 1/2 \} \), \( q_{ij} = \# \{ k : x_{ik} \neq x_{jk} \neq 1/2 \} \), thus \( \sum_{i,j} h_{ij} = \frac{2}{9} ns \) and \( \sum_{i,j} q_{ij} = \frac{2}{9} ns \). The discrepancy for the symmetric design \( U = \left( X, X^* \right) \) is
\[
[CD(U)]^2 = [CD(X)]^2 - \frac{1}{2n^2} \sum_{j=1}^{r} \left( 4/3 \right)^{h_j} + \frac{1}{2n^2} \sum_{j=1}^{r} \left( 4/3 \right)^{q_j}.
\]

Furthermore,
\[
[CD(X)]^2 + \frac{s}{9n} - \frac{s}{9n} \left( 4/3 \right)^3 \leq [CD(U)]^2 \leq [CD(X)]^2 + \frac{s}{9n} \left( 4/3 \right)^3 - \frac{s}{9n}.
\]

(3)

Corollary 1 indicates that the symmetric design U's discrepancy can be expressed by the discrepancy of the initial design X. Furthermore, the initial design X is more close to be uniform, both the lower bound and upper bound of discrepancy interval of U is closer. The lower bound in Corollary 1 can be used as a bench mark when searching for uniform symmetric designs.

**Partial Fold Over Plan for Uniform Design**

For any initial design \( d = (x_{ij})_{ns \times r}, 0 < x_{ij} < 1 \), Define a fold over plan by \( \delta = (\delta_1, \delta_2, \ldots, \delta_r), \delta_i = 1 \) if the \( i \)th column of \( d \) is reversed, otherwise \( \delta_i = 0 \). For a initial uniform design \( d \) and fold over plan \( \delta \), the fold over design denoted by \( d_\delta = (x_{ij}^\delta)_{ns \times r}, \) then
\[
x_{ij}^\delta = (-1)^{\delta_i} x_{ij} + \delta_j = \begin{cases} 1-x_{ij} & \text{if } \delta_j = 1 \\ x_{ij} & \text{if } \delta_j = 0 \end{cases}
\]

(4)

The full design obtained by joining the runs in the fold over design \( d_\delta \) to those of the initial design \( d \) is called the combined design, denote by \( d(\delta) \), that is \( d(\delta) = \left( \begin{array}{c} d \\ d_\delta \end{array} \right) \). If \( \delta = (1,1,\ldots,1) \), it is the full
fold-over plan discussed in Section 2.

Define $\Omega = \{ \delta = (\delta_1, \delta_2, \cdots, \delta_s), \delta = 0 \text{ or } 1 \} \), under a fold over plan $\delta \in \Omega$, the centered $L_2$ discrepancy of the combined design $d(\delta)$, denoted by $CD(d(\delta))$ can be found to be

$$[CD(d(\delta))]^2 = \left( \frac{13}{12} \right)^2 - \frac{2}{n} \sum_{k=1}^{n} \prod_{j=1}^{s} \left( 1 + \frac{1}{2} \left| x_{ki} - \frac{1}{2} \right| - \frac{1}{2} \left| x_{ji} - \frac{1}{2} \right| \right)$$

$$+ \frac{1}{2n^2} \sum_{k=1}^{n} \sum_{j=1}^{s} \prod_{i=1}^{m} \left[ 1 + \frac{1}{2} \left| x_{ki} - \frac{1}{2} \right| + \frac{1}{2} \left| x_{ji} - \frac{1}{2} \right| - \frac{1}{2} \left| x_{ki} - x_{ji} \right| \right]$$

$$+ \frac{1}{2n^2} \sum_{k=1}^{n} \sum_{j=1}^{s} \prod_{i=1}^{m} \left[ 1 + \frac{1}{2} \left| x_{ki} - \frac{1}{2} \right| + \frac{1}{2} \left( x_{ji} - \frac{1}{2} \right) - \frac{1}{2} \left| x_{ki} - x_{ji} \right| \right].$$

Given the original design $d$, the optimal fold over plan $\delta^*$ of $d$ in this paper is defined as

$$\delta^* = \arg\min_{\delta \in \Omega} [CD(d(\delta))]^2.$$

By the above formula, the optimal foldover plan for any uniform design $d$ can be constructed through an algorithm, as shown in Example 3.1 below.

**Example 3.1:** Take uniform design $U(8; 8^7)$ (Runs 1-8 in Table 2) as an example. The full foldover plan, as shown on the left portion of Table 2, the partial foldover plan is shown on the right portion of Table 2. All the foldover plans ($2^7 = 128$) can help to reduce the discrepancy, and the optimal foldover plan is $\delta^* = (1, 0, 1, 1, 0, 1, 1)$. Compare with the full foldover plan, their discrepancies are almost identical (0.0614 versus 0.0620).

**Example 3.2** Consider a design $U(3; 3^2)$, given in the top portion of Table 3 with $n = 3; s = 12$. The full foldover plan is shown on the left portion of Table 3, while the optimal foldover plan is shown on the right portion of Table 3. This example has been discussed in Elsawah and Qin (2016)[2] (Example 5.2). They discussed the optimal foldover plan by permutation method, while here we discuss it by our new method. Their optimal foldover plan is different from ours, but the discrepancy of corresponding combined design are the same of 1.0515, obtains their lower bound.

| No. | Full fold-over plan | Optimal foldover plan |
|-----|---------------------|-----------------------|
| 1   | 0 0 1 2 2 0 1 0 1 2 0 | 0 0 1 2 2 0 1 0 1 2 0 |
| 2   | 1 2 2 0 1 1 0 2 2 0 1 | 1 2 2 0 1 1 0 2 2 0 1 |
| 3   | 2 1 0 2 1 0 2 1 0 1 2 | 2 1 0 2 1 0 2 1 0 1 2 |
| 4   | 2 2 1 1 0 0 2 1 2 1 0 2 | 2 2 1 1 0 0 2 1 2 1 0 2 |
| 5   | 1 0 2 2 1 1 0 2 0 2 1 | 1 0 2 2 1 1 0 2 0 2 1 |
| 6   | 0 1 2 0 1 2 0 0 1 2 1 0 | 0 1 2 0 1 2 0 0 1 2 1 0 |
| Fold-over plan | (1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1) | (0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1) |
| CD value | 1.185205 | 1.051461 |

Compared with partial fold over plan, full fold over plan on uniform designs can produce a symmetric design and its discrepancy will not too bad. Both full foldover and partial foldover, we have the best design for each stage.

**Concluding Remarks**

In this article we investigated the optimal foldover plans for uniform designs in terms of centered $L_2$ discrepancy. Followup experiments is an important issue in both the design theory and practice. How to get a good followup plan is controversial problem. Many researchers did permutation method, we
here did reection method here. It reduce the computations substantially for any type of uniform design. For a uniform design of n runs and s q-level factors, the permutation method need to compare \((q-1)\) different designs to find the optimal fold over plan, while by our method only \(2^s\) different designs need to compare. The proposed method may conclude to a less effective combined design than the permutation method. Example 3.2 shows they lead to different optimal combined designs, but they have the same discrepancy. For a \(n\) run uniform design, high level of each factor is always preferred to lower level of each factor. Under this circumstance, Our method is more implementable.

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