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Projection uniformity under mixture discrepancy

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ABSTRACT

The objective of this paper is to discuss the issue of projection uniformity under mixture discrepancy (MD). The uniformity pattern (UP) and minimum projection uniformity criterion are defined for two- and three-level designs under MD. It is shown that the projection uniformity under MD is better than that of other discrepancies, and there is a linear relationship between UP and generalized word-length pattern. Moreover, it is also shown that the foldover technique can increase uniformity resolution. The lower bounds of projection discrepancy for foldover designs and more general follow-up designs are also obtained for two-level designs. For three-level designs, the UP is defined through the average projection discrepancy based on level permutation of factors and its property is also discussed.

1. Introduction

Uniform design (UD) has been widely used in physical and computer experiments (see Fang et al., 2006). The main idea of UD is to scatter the design points uniformly on the experimental domain. As a measure of uniformity, discrepancy plays a key role in UD and various discrepancies have been proposed by using the tool of reproducing kernel Hilbert space, such as centered L_2-discrepancy (CD, Hickernell, 1998a), wrap-around L_2-discrepancy (WD, Hickernell, 1998b), discrete discrepancy (DD, Liu and Hickernell, 2002) and mixture discrepancy (MD, Zhou et al., 2013).

Two- and three-level factorials are widely used and it is meaningful to consider the projection property under an assumption of effect sparsity. The projection uniformity criterion favors designs with the smallest projection discrepancy value of different dimensions. Fang and Qin (2005) proposed the uniformity pattern (UP) and minimum projection uniformity (MPU) criterion under CD, and showed that it is equivalent to generalized minimum aberration (GMA) for two-level designs. The UP is defined through the projection discrepancy and can measure the projection uniformity of different dimensions. Zhang and Qin (2006) established the relationship between UP with other criteria under CD for two-level designs. Qin et al. (2012) and Wang and Qin (2017) discussed UP for q-level and mixed-level designs under DD, respectively. However, Zhou et al. (2008) pointed out the shortcoming of DD for constructing UDs with multi-level factors. In addition, Gou et al. (2018) studied UP and lower bounds of projection uniformity measure for follow-up designs under CD.

However, Zhou et al. (2013) showed that WD does not have the sensitiveness on a shift for one or more dimensions and CD has the problem with curse of dimensionality, and MD retains good properties of CD and WD and overcomes the unreasonable phenomena for them. Then, we focus on MD in this paper, since MD is a more suitable choice as a uniformity measure. It is necessary to investigate more properties of MD. Ke et al. (2015) obtained lower bounds of two- and three-level designs under MD. Zhou and Xu (2014) discussed level permutations and showed the relationship between average

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discrepancy value and generalized word-length pattern (GWP). Elsawah and Qin (2016) took two- and three-level factorials as the initial designs and assessed the optimal foldover plans under MD.

In this paper, we investigate the projection properties of factorials under MD. We discuss the UP and related criteria for two- and three-level designs, and give the linear relationship between UP and GWP. Therefore, we establish a statistical justification of UP and MPU. Moreover, we calculate the lower bounds of the projection discrepancy for two-level foldover designs and extend corresponding results to follow-up designs.

This paper is organized as follows. Section 2 defines the projection discrepancy and related UP under MD for two-level designs. Section 3 discusses the projection discrepancy and corresponding lower bounds for foldover designs. Section 4 gives the lower bounds of projection discrepancy for general follow-up designs. Section 5 defines the average projection discrepancy to form UP for three-level designs. Finally conclusion is given in Section 6.

2. Uniformity pattern under MD

Denote $\mathcal{D}(n; q^s)$ as all the designs with n runs, s factors and q levels, $0, 1, \ldots, q-1$. Then, each design $D = (u_{ij}) \in \mathcal{D}(n; q^s)$ can be transformed onto $C^s = [0, 1]^s$ by $x_{ij} = (2u_{ij} + 1)/(2q), i = 1, \ldots, n; j = 1, \ldots, s$. Let $u \subset \{1, \ldots, s\}$ be the index of the factors of interest, $C^u = [0, 1]^u$ be the unit cube in the coordinates indexed by u, and D_u be the projection of the design D onto C^u. Zhou et al. (2013) gave the definition of MD by $MD(D, \mathcal{K}) = \left\{\int_{C^{2s}} \mathcal{K}(\boldsymbol{x}, \boldsymbol{y})d\boldsymbol{x}d\boldsymbol{y} - \frac{2}{n}\sum_{i=1}^{n} \int_{C^s} \mathcal{K}(\boldsymbol{x}_i, \boldsymbol{y})d\boldsymbol{y} + \frac{1}{n^2}\sum_{i,j=1}^{n}\mathcal{K}(\boldsymbol{x}_i, \boldsymbol{y}_j)\right\}^{1/2}$, where the kernel function is $\mathcal{K}(\boldsymbol{x}, \boldsymbol{y}) = \prod_{j=1}^{s}[1+k_j(x_j, y_j)]$ with

$$k_j(x_j, y_j) = \frac{7}{8} - \frac{1}{4}\left|x_j - \frac{1}{2}\right| - \frac{1}{4}\left|y_j - \frac{1}{2}\right| - \frac{3}{4}\left|x_j - y_j\right| + \frac{1}{2}\left|x_j - y_j\right|^2. \tag{1}$$

In this section, we consider the projection property of two-level factorials under MD. As similar as Hickernell and Liu (2002), we define the u-projection discrepancy of MD, $MD_u(D)$, as follows,

$$[MD_u\,(D, \mathcal{K})]^2 = \prod_{j\in u}\int_{[0,1)^2} k_j(x, y)dxdy - \frac{2}{n}\sum_{i=1}^{n}\prod_{j\in u}\int_{[0,1)} k_j(x_{ij}, y)dy + \frac{1}{n^2}\sum_{i,k=1}^{n}\prod_{j\in u} k_j(x_{ij}, x_{kj}). \tag{2}$$

Then the formula of $[MD_u(D)]^2$ is as follows:

$$\begin{aligned}[MD_u(D)]^2 = {} & \left(\frac{7}{12}\right)^{|u|} - \frac{2}{n}\sum_{i=1}^{n}\prod_{j\in u}\left(\frac{2}{3} - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right| - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right|^2\right) \\ & + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{k=1}^{n}\prod_{j\in u}\left[\frac{7}{8} - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right| - \frac{1}{4}\left|x_{kj} - \frac{1}{2}\right| - \frac{3}{4}\left|x_{ij} - x_{kj}\right| + \frac{1}{2}\left|x_{ij} - x_{kj}\right|^2\right],\end{aligned} \tag{3}$$

where $x_{ij}, j \in u$ are the components of the ith point of D_u, and $|u|$ means the cardinality of subset u.

Define

$$[I_i(D)]^2 = \sum_{|u|=i}[MD_u(D)]^2, \tag{4}$$

which measures the overall uniformity of D in all the i-subdimension. Obviously, $\sum_{i=1}^{s}[I_i(D)]^2 = [MD(D)]^2$. Moreover, denote $AI_i(D) = I_i(D)/\binom{s}{i}$, which measures the average uniformity of D on C^u with $|u| = i$.

For illustrating the reasonableness of the projection uniformity under MD, we randomly generate 100 designs in $\mathcal{D}(20, 4^s)$, $s = 4, 8, 12, 16$, and obtain the corresponding vectors $(I_1(D), \ldots, I_s(D))$ and $(AI_1(D), \ldots, AI_s(D))$. Moreover, we calculate the corresponding vectors under CD and WD of those 100 designs similarly. Each vector is normalized such that the summation of the elements of each vector equals 1, and we obtain the mean of each element of the 100 vectors $(I_1(D), \ldots, I_s(D))$ and the 100 vectors $(AI_1(D), \ldots, AI_s(D))$. Fig. 1 shows the mean of these vectors. From Fig. 1(e)–(h), it is known that CD and WD focus on the low-dimension projection and those values of the mean vectors decrease exponentially with the increase of i. However, the mean vectors of MD uniformly scatter in every projection dimension. For the designs with other levels, they have similar results. It is expected that the UD may have the same weight for each low-dimension, as the same as the true uniform distribution. Thus, MD may be a better choice in the sense of the uniformity of subdimension projection. Therefore, we should study more properties of MD such as the UP under MD, which is the main content in this paper.

For any design $D \in \mathcal{D}(n; 2^s)$, define

$$E_k(D) = \frac{1}{n}\left|\{(c, d) : c, d \text{ are rows of } D,\ \ d_H(c, d) = k\}\right|, \text{for } k = 0, 1, \ldots, s, \tag{5}$$

where $d_H(c, d)$ is the Hamming distance between two runs c and d. The vector $(E_0(D), \ldots, E_s(D))$ is called the *distance distribution* of D in the literature. The next lemma shows the link between $[MD_u(D)]^2$ and the distance distribution for two-level designs.

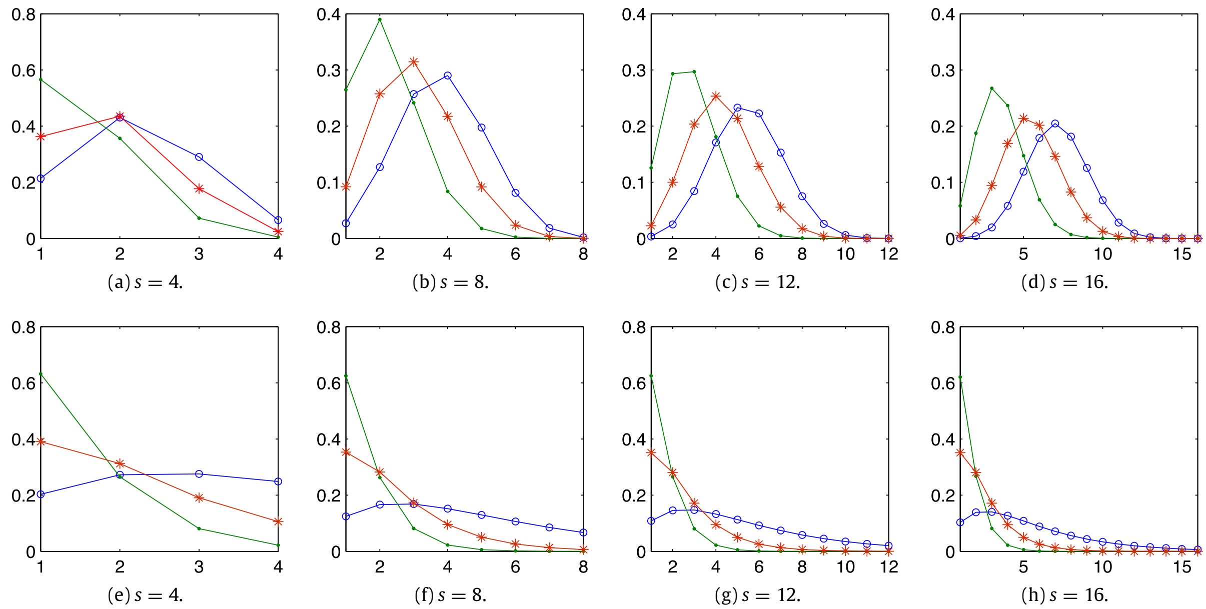

Fig. 1. (a)–(d): the mean vector of $(I_1(D), \ldots, I_s(D))$ for $\mathcal{D}(20, 4^s)$; (e)–(h): the mean vector of $(AI_1(D), \ldots, AI_s(D))$ for $\mathcal{D}(20, 4^s)$. The lines '$-\cdot$', '$-*$' and '$-\circ$' denote for CD, WD and MD, respectively.

Lemma 1. *For any design $D \in \mathcal{D}(n, 2^s)$ and any nonempty subset u of $\{1, \ldots, s\}$ we have*

$$[MD_u(D)]^2 = \left(\frac{7}{12}\right)^{|u|} - 2\left(\frac{113}{192}\right)^{|u|} + \frac{1}{n}\left(\frac{3}{4}\right)^{|u|} \sum_{i=0}^{|u|} \left(\frac{2}{3}\right)^{i} E_i\left(D_u\right), \tag{6}$$

where D_u is the projection of D onto C^u.

Proof. According to formulas (3) and (5), we have

$$\begin{aligned}
[MD_u(D)]^2 &= \left(\frac{7}{12}\right)^{|u|} - 2\left(\frac{113}{192}\right)^{|u|} + \left(\frac{3}{4}\right)^{|u|} \frac{1}{n^2} \sum_{i=1}^{n} \sum_{k=1}^{n} \prod_{j\in u} \left[1 - \left|x_{ij} - x_{kj}\right| + \frac{2}{3}\left|x_{ij} - x_{kj}\right|^2\right] \\
&= \left(\frac{7}{12}\right)^{|u|} - 2\left(\frac{113}{192}\right)^{|u|} + \left(\frac{3}{4}\right)^{|u|} \frac{1}{n^2} \sum_{i=1}^{n} \sum_{k=1}^{n} \mathbf{1}^{|u|-d_H(d_i^u, d_k^u)} \left(\frac{2}{3}\right)^{d_H(d_i^u, d_k^u)} \\
&= \left(\frac{7}{12}\right)^{|u|} - 2\left(\frac{113}{192}\right)^{|u|} + \frac{1}{n}\left(\frac{3}{4}\right)^{|u|} \sum_{i=0}^{|u|} \left(\frac{2}{3}\right)^{i} E_i\left(D_u\right),
\end{aligned}$$

which completes the proof.

Moreover, denote an orthogonal array (OA) of strength t with n runs and s factors by $OA(n, s, t)$. If D is an $OA(n, s, t)$, then for $1 \le j \le t$ and $|u| = j$, all possible 2^j level combinations among any j columns of D appear equally often. It is easy to obtain that for a given row c_0, $|\{(c_0, d) : d_H(c_0, d) = i\}| = \binom{j}{i} \frac{n}{2^j}$, representing the number of row d which has i different positions from the row c_0. Thus, we have

$$\frac{1}{n}\left(\frac{3}{4}\right)^{j} \sum_{i=0}^{j} \left(\frac{2}{3}\right)^{i} E_i(D_u) = \frac{1}{n^2}\left(\frac{3}{4}\right)^{j} \sum_{i=0}^{j} \left[\left(\frac{2}{3}\right)^{i} \binom{j}{i} \frac{n}{2^j} \times n\right] = \left(\frac{3}{8}\right)^{j} \sum_{i=0}^{j} \binom{j}{i} \left(\frac{2}{3}\right)^{i} = \left(\frac{3}{8}\right)^{j} \left(\frac{5}{3}\right)^{j} = \left(\frac{5}{8}\right)^{j}, \tag{7}$$

and substituting (7) into (6), we have $[MD_u(D)]^2 = \Lambda$, where $\Lambda = \left(\frac{7}{12}\right)^j - 2\left(\frac{113}{192}\right)^j + \left(\frac{5}{8}\right)^j$, which is also the smallest u-projection discrepancy value in $\mathcal{D}(n, 2^j)$, since Chen et al. (2015) showed that two-level full design is a UD under MD. Moreover, from Eq. (4), $[I_j(D)]^2 = \binom{s}{j} \Lambda$, for $1 \le j \le t$. When $j > t$, D_u cannot be a full design, therefore it cannot obtain the smallest discrepancy value, *i.e.*, $[I_j(D)]^2 > \binom{s}{j}\Lambda$. For any $D \in \mathcal{D}(n, 2^s)$, define

$$MI_k(D) = [I_k(D)]^2 - \binom{s}{k}\left[\left(\frac{7}{12}\right)^k - 2\left(\frac{113}{192}\right)^k + \left(\frac{5}{8}\right)^k\right], 1 \le k \le s. \tag{8}$$

We call the vector

$$(MI_1(D), \dots, MI_s(D)) \tag{9}$$

as the *uniformity pattern* of the two-level design D. Define the *uniformity resolution* of D be the smallest integer k such that $MI_k(D) > 0$ in its UP. Let r be the smallest integer such that $MI_r(D_1) \neq MI_r(D_2)$ and D_1 is said to have less projection uniformity than D_2 if $MI_r(D_1) < MI_r(D_2)$. D has minimum projection uniformity (MPU) if no other design has less projection uniformity than it.

Based on the above discussion, we have the following relationship between UP and strength.

Theorem 1. *For any design $D \in \mathcal{D}(n, 2^s)$, D is of strength t if and only if $MI_k(D) = 0$, $1 \le k \le t$ and $MI_{t+1}(D) \neq 0$.*

Theorem 1 shows that the uniformity resolution is equivalent to the strength in orthogonal designs. Furthermore, for a design $D \in \mathcal{D}(n; 2^s)$, define $A_j(D) = \frac{1}{n}\sum_{k=0}^{s} P_j(k; s, 2)E_k(D)$, for $j = 1, \dots, s$ and $P_j(k; s, 2) = \sum_{r=0}^{j}(-1)^r \binom{k}{r}\binom{s-k}{j-r}$ is the Krawtchouk polynomial, $\binom{y}{z}$=0 if $y < z$. Then $(A_1(D), \dots, A_s(D))$ is the GWP and it measures the degree of aliasing and indicates the statistical inference ability of a design. The GMA criterion is to sequentially minimize $A_j(D)$ for $j = 1, \dots, s$. In addition, for every m column of D, $(D_{l_1}, D_{l_2}, \dots, D_{l_m})$, define $B_{l_1\dots l_m}(D) = \sum_{\alpha_1,\dots,\alpha_m}\left(n^{l_1\dots l_m}_{\alpha_1\dots\alpha_m} - n/2^m\right)^2$, where $n^{l_1\dots l_m}_{\alpha_1\dots\alpha_m}$ is the number of runs in which $(D_{l_1}, D_{l_2}, \dots, D_{l_m})$ takes the level combination $(\alpha_1 \dots \alpha_m)$, and the summation is taken over all 2^m level combinations. Define $B_m(D) = \sum_{1\le l_1<\dots<l_m\le s} B_{l_1\dots l_m}(D)/\binom{s}{m}$, for $1 \le m \le s$. $B_m(D) = 0$ means the design D is an OA of strength m. The balance pattern is defined as the vector $(B_1(D), \dots, B_s(D))$. Then the connection between $MI_j(D)$ and $A_j(D)$ is as follows.

Theorem 2. *For any design $D \in \mathcal{D}(n, 2^s)$, there exists the linear relationship between MI_k and A_k, $1 \le k \le s$,*

$$MI_k(D) = \left(\frac{5}{8}\right)^k \sum_{v=1}^{k}\left(\frac{1}{5}\right)^v \binom{s-v}{s-k} A_v(D). \tag{10}$$

Proof. From the formulas (4) and (6) and (8), we have

$$\begin{aligned} MI_k(D) &= \sum_{|u|=k}\left[\frac{1}{n}\left(\frac{3}{4}\right)^k \sum_{i=0}^{k}\left(\frac{2}{3}\right)^i E_i(D_u) - \left(\frac{5}{8}\right)^k\right] = \sum_{|u|=k}\left[\left(\frac{3}{8}\right)^k \sum_{v=0}^{k}\left(\sum_{i=0}^{k}\left(\frac{2}{3}\right)^i P_i(v; k, 2)\right)A_v(D_u) - \left(\frac{5}{8}\right)^k\right] \\ &= \sum_{|u|=k}\left[\left(\frac{3}{8}\right)^k \sum_{v=0}^{k}\left(\frac{5}{3}\right)^{k-v}\left(\frac{1}{3}\right)^v A_v(D_u) - \left(\frac{5}{8}\right)^k\right] = \sum_{|u|=k}\left[\left(\frac{5}{8}\right)^k \sum_{v=1}^{k}\left(\frac{1}{5}\right)^v A_v(D_u)\right], \end{aligned} \tag{11}$$

according to properties of the Krawtchouk polynomial, *i.e.* $E_\omega(D) = \frac{n}{2^s}\sum_{v=0}^{s} P_\omega(v; s, 2)A_v(D)$ and for any integer s, $0 \le j \le s$, and real $a > 0$, $\sum_{i=0}^{s} a^i P_i(j; s, 2) = (1+a)^{s-j}(1-a)^j$. Moreover, It was showed that $B_v(D) = \frac{n^2}{2^s}A_v(D)$ and $\sum_{|u|=k} 2^k B_v(D_u) = 2^s\binom{s-v}{s-k}B_v(D)$, see Fang et al. (2002) and Wang and Qin (2017). Then we can get the formula $\sum_{|u|=k} A_v(D_u) = \binom{s-v}{s-k}A_v(D)$. Hence, formula (11) can be simplified as formula (10), which completes the proof.

Theorem 2 shows that MPU (uniformity resolution) is almost equivalent to GMA (resolution) for two-level factorials under MD. Here, an example is shown for the reasonableness of UP.

Example 1. Consider three designs in $\mathcal{D}(12; 2^5)$, as shown in Table 1. The corresponding GWP and UP of D_1, D_2 and D_3 are calculated. Observe that $MI_k(D_1) = MI_k(D_2)$ for $k < 5$, and $MI_5(D_1) > MI_5(D_2)$, and the GWP of D_1 and D_2 has similar result, hence D_2 has better projection uniformity than D_1. Moreover, $MI_k(D_1) = MI_k(D_2) = 0$ for $k < 3$, then both designs have uniformity resolution III. Obviously, D_3 has the worst projection uniformity among the three designs with regard to MPU criterion. Furthermore, the MD-values of D_1, D_2 and D_3 are 1.05655, 1.05654 and 1.1401, respectively. Then, the rank of MD-values is consistent with the rank of projection uniformity.

3. Uniformity pattern for foldover design

In order to release the aliasing in two-level designs, a standard strategy is to augment a foldover design of the same size by reversing the plus and minus signs of one or more columns of the original design. Detailed discussion can be found in Wu

Table 1
Three designs in $\mathcal{D}(12; 2^5)$ and the corresponding GWP and UP.

D_1					D_2					D_3				
1	1	0	1	1	1	1	0	1	1	1	0	0	1	0
0	1	1	0	0	0	1	1	0	1	1	0	1	1	0
1	0	1	1	0	1	0	1	1	0	1	1	0	1	1
0	1	0	1	0	0	1	0	1	1	1	1	1	1	1
0	0	1	0	1	0	0	1	0	1	1	0	0	0	0
0	0	0	1	1	0	0	0	1	0	1	0	0	1	1
1	0	0	0	1	1	0	0	0	1	0	1	1	0	0
1	1	0	0	0	1	1	0	0	0	0	1	1	1	1
1	1	1	0	1	1	1	1	0	0	0	1	1	0	1
0	1	1	1	1	0	1	1	1	0	0	1	0	0	1
1	0	1	1	0	1	0	1	1	1	0	0	1	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Design	GWP					UP				
	A_1	A_2	A_3	A_4	A_5	MI_1	MI_2	MI_3	MI_4	MI_5
D_1	0	0	10/9	5/9	4/9	0	0	0.0022	0.0028	0.00095
D_2	0	0	10/9	5/9	0	0	0	0.0022	0.0028	0.00093
D_3	0	4/3	0	1/3	0	0	0.0208	0.0391	0.0245	0.0051

and Hamada (2000) and Box et al. (2005). In this section, we will calculate the projection discrepancy value of the two-level combined design and compare the UP between original design and combined design. In addition, we will show the lower bound of the combined design's projection discrepancy.

For two-level factorials, define $\Gamma = \{(\gamma_1, \ldots, \gamma_s) \mid \gamma_j = 0, 1; 1 \le j \le s\}$, then for any $\gamma = (\gamma_1, \ldots, \gamma_s) \in \Gamma$, it represents a foldover plan for any two-level balanced design $D \in \mathcal{B}(n, 2^s)$ where each factor takes values from the set $\{0, 1\}$ equally often. According to a foldover plan, the foldover design is a vector denoted by $D_f = (f^1, \ldots, f^s)$, where $f^j = (f_{1j}, \ldots, f_{nj})' = (u_{1j}+\gamma_j, \ldots, u_{nj}+\gamma_j)'(mod\, 2)$. Thus, each foldover design is generated by a foldover plan. The full design obtained by augmenting the foldover design D_f to the original design D is called combined design, denoted as $D_c = (D', D_f')'$. And the set of all two-level combined designs is denoted by $\mathcal{C}(n, 2^s)$.

Let u represent any nonempty subset of $\{1, \ldots, s\}$ and Γ_w be the set of all elements $\gamma \in \Gamma$ such that γ exactly has w nonzero components among $\{\gamma_j, j \in u\}$. For any foldover plan $\gamma = (\gamma_1, \ldots, \gamma_s) \in \Gamma_w$, let $N_w^\gamma = \{v \mid \gamma_v \ne 0, v \in u\}$ be of cardinality w, and $\overline{N}_w^\gamma = u - N_w^\gamma$. Let R_u and $\overline{R}_u$ respectively be the subdesigns with the column groups N_w^γ and $\overline{N}_w^\gamma$ in the projected original design D_u, and R_{uf} be the subdesign with the column groups N_w^γ in the projected foldover design D_{uf} corresponding to γ.

For any u and any foldover plan $\gamma = (\gamma_1, \ldots, \gamma_s) \in \Gamma_w$, the u-projection discrepancy value of the two-level combined design D_c^w under MD, denoted by $MD_u(D_c^w)$, can be calculated as follows.

Lemma 2. *For any two-level combined design $D_c^w \in \mathcal{C}(n, 2^s)$ and any nonempty subset u of $\{1, \ldots, s\}$, we have*

$$\left[MD_u(D_c^w)\right]^2 = \left(\frac{7}{12}\right)^{|u|} - 2\left(\frac{113}{192}\right)^{|u|} + \left(\frac{3}{4}\right)^{|u|} \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{k=1}^{n} \left(\frac{2}{3}\right)^{d_H(d_i^{D_u}, d_k^{D_u})}$$
$$+ \left(\frac{3}{4}\right)^{|u|} \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{k=1}^{n} \left(\frac{2}{3}\right)^{d_H(d_i^{\overline{R}_u}, d_k^{\overline{R}_u}) + d_H(d_i^{R_u}, d_k^{R_{uf}})}, \tag{12}$$

where $d_H(d_i^{D_u}, d_k^{D_u})$ and $d_H(d_i^{\overline{R}_u}, d_k^{\overline{R}_u})$ are the Hamming distances for the ith row and the kth row of the designs D_u and $\overline{R}_u$, respectively, and $d_H(d_i^{R_u}, d_k^{R_{uf}})$ is the Hamming distance for the ith row of the design R_u and the kth row of the design R_{uf}.

Proof. As similar as the proof of Theorem 1 of Elsawah and Qin (2016), we can obtain that

$$\left[MD_u(D_c^w)\right]^2 = \left(\frac{7}{12}\right)^{|u|} - \frac{2}{n} \sum_{i=1}^{n} \prod_{j \in u} \Delta_1 + \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{k=1}^{n} \prod_{j \in u} \Delta_{ikj} + \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{k=1}^{n} \prod_{j \in u} \Delta_{ikj}(\gamma_j),$$

where $\Delta_{ikj} = \frac{7}{8} - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right| - \frac{1}{4}\left|x_{kj} - \frac{1}{2}\right| - \frac{3}{4}\left|x_{ij} - x_{kj}\right| + \frac{1}{2}\left|x_{ij} - x_{kj}\right|^2$, $\Delta_{ikj}(\gamma_j) = \frac{7}{8} - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right| - \frac{1}{4}\left|x_{kj} - \frac{1}{2}\right| - \frac{3}{4}\left|x_{ij} - x_{kj}^{(\gamma_j)}\right| + \frac{1}{2}\left|x_{ij} - x_{kj}^{(\gamma_j)}\right|^2$, $\Delta_1 = \frac{2}{3} - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right| - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right|^2$, $x_{kj}^{(\gamma_j)} = \frac{2(u_{kj}+\gamma_j)(\mathrm{mod}\ 2)+1}{4}$, $x_{ij} = \frac{2u_{ij}+1}{4}$ *and* $u_{ij} \in \{0, 1\}$. Then

$$\begin{aligned}
\left[MD_u(D_c^w)\right]^2 &= \left(\frac{7}{12}\right)^{|u|} - 2\left(\frac{113}{192}\right)^{|u|} + \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{k=1}^{n}\prod_{j\in u}\Delta_{ikj} + \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{k=1}^{n}\prod_{j\in \bar{N}_w^{\gamma}}\Delta_{ikj}\prod_{j\in N_w^{\gamma}}\Delta_{ikj}(\gamma_j)\\
&= \left(\frac{7}{12}\right)^{|u|} - 2\left(\frac{113}{192}\right)^{|u|} + \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{k=1}^{n}\left(\frac{3}{4}\right)^{|u|-d_H(d_i^{D_u},d_k^{D_u})}\left(\frac{1}{2}\right)^{d_H(d_i^{D_u},d_k^{D_u})} +\\
&\quad \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{k=1}^{n}\left(\frac{3}{4}\right)^{|u|-w-d_H(d_i^{\bar{R}_u},d_k^{\bar{R}_u})}\left(\frac{1}{2}\right)^{d_H(d_i^{\bar{R}_u},d_k^{\bar{R}_u})}\left(\frac{3}{4}\right)^{w-d_H(d_i^{R_u},d_k^{R_{uf}})}\left(\frac{1}{2}\right)^{d_H(d_i^{R_u},d_k^{R_{uf}})},
\end{aligned}$$

and after some simple transformation, we can get the result and complete the proof.

Comparing Lemma 1 with Lemma 2, we can find that the last term of $[MD_u(D)]^2$ and $[MD_u(D_c^w)]^2$ is different. It is easy to check that the set $\{d_H(d_i^u, d_k^u), i, k = 1, \ldots, n\}$ is equal to $\{d_H(d_i^{\bar{R}_u}, d_k^{\bar{R}_u}) + d_H(d_i^{R_u}, d_k^{R_{uf}}), i, k = 1, \ldots, n\}$ if D is an $OA(n, s, t)$ and $1 \le |u| \le t$. Then $[MD_u(D)]^2 = [MD_u(D_c^w)]^2$. Thus, we can obtain the following result.

Theorem 3. *For any design $D \in \mathcal{D}(n, 2^s)$ with strength t, $MI_k(D_c^w) = 0$ under any foldover plan $\gamma = (\gamma_1, \ldots, \gamma_s) \in \Gamma_w$, $1 \le k \le t$.*

According to Theorem 3, the combined design may have higher uniformity resolution comparing with the original design if the strength becomes higher under some special foldover plan. A commonly used foldover strategy for a resolution III design involves reversing the signs of all factors, and the resulting combined design has resolution IV. If the resulting combined design D_c^w has resolution IV, we can obtain $MI_k(D_c^w) = 0, k \le 3$ and the uniformity resolution is four according to Theorem 1. Moreover, MPU can also be used as a criteria to find the optimal foldover plan γ^* such that $D_c^w(\gamma^*)$ has minimum projection uniformity according to Theorem 2.

Additionally, according to Lemma 2, we can also obtain the lower bounds of u-projection discrepancy and projection discrepancy $[I_k(D_c^w)]^2$ for the combined design as follows.

Theorem 4. *For any two-level combined design $D_c^w \in \mathcal{C}(n, 2^s)$, we have $[MD_u(D_c^w)]^2 \ge LB_{1u}$, where*

$$\begin{aligned}
LB_{1u} =& \left(\frac{7}{12}\right)^{|u|} - 2\left(\frac{113}{192}\right)^{|u|} + \left(\frac{3}{4}\right)^{|u|}\frac{1}{2n}\left[1 + \left(\frac{2}{3}\right)^{w}\right]\\
&+ \left(\frac{3}{4}\right)^{|u|}\frac{1}{2n^2}\left[\left(\frac{2}{3}\right)^{\alpha_1}\left(p_1 + \frac{2}{3}q_1\right) + \left(\frac{2}{3}\right)^{\alpha_2}\left(p_2 + \frac{2}{3}q_2\right)\right]
\end{aligned} \tag{13}$$

and $n = 2l$, $\alpha_1 = \left\lfloor \frac{|u|(n-l)}{n-1} \right\rfloor$, $p_1\alpha_1 + q_1(\alpha_1+1) = n|u|(n-l)$, $p_1+q_1 = q_2+q_2 = n(n-1)$, $\alpha_2 = \left\lfloor \frac{|u|(n-l)-w}{n-1} \right\rfloor$, $p_2\alpha_2+q_2(\alpha_2+1) = n|u|(n-l) - nw$, and $\lfloor\delta\rfloor$ means the largest integer contained in δ.

Proof. According to the definition of $d_H(\cdot, \cdot)$ in Lemma 2, it is easy to check that $d_H(d_i^{D_u}, d_i^{D_u}) = 0$, $d_H(d_i^{\bar{R}_u}, d_i^{\bar{R}_u}) = 0$ and $d_H(d_i^{R_u}, d_i^{R_{uf}}) = w$. Thus, we can transform formula (12) into

$$\begin{aligned}
[MD_u(D_c^w)]^2 =& \left(\frac{7}{12}\right)^{|u|} - 2\left(\frac{113}{192}\right)^{|u|} + \left(\frac{3}{4}\right)^{|u|}\frac{1}{2n}\left[1 + \left(\frac{2}{3}\right)^{w}\right]\\
&+ \left(\frac{3}{4}\right)^{|u|}\frac{1}{2n^2}\sum_{i=1}^{n}\sum_{k\ne i}^{n}\left(\frac{2}{3}\right)^{d_H(d_i^{D_u},d_k^{D_u})} + \left(\frac{3}{4}\right)^{|u|}\frac{1}{2n^2}\sum_{i=1}^{n}\sum_{k\ne i}^{n}\left(\frac{2}{3}\right)^{d_H(d_i^{\bar{R}_u},d_k^{\bar{R}_u})+d_H(d_i^{R_u},d_k^{R_{uf}})}.
\end{aligned} \tag{14}$$

From Lemma 1 of Elsawah and Qin (2016), we can obtain that $\sum_{i=1}^{n}\sum_{k\ne i}^{n} d_H(d_i^{D_u}, d_k^{D_u}) = n|u|(n-l)$, $\sum_{i=1}^{n}\sum_{k\ne i}^{n} d_H(d_i^{\bar{R}_u}, d_k^{\bar{R}_u}) = n(|u|-w)(n-l)$ and $\sum_{i=1}^{n}\sum_{k\ne i}^{n} d_H(d_i^{R_u}, d_k^{R_{uf}}) = nw(n-l-1)$. Thus, from Lemma 2 of Elsawah and Qin (2016), we know that $\sum_{i=1}^{n}\sum_{k\ne i}^{n}\left(\frac{2}{3}\right)^{d_H(d_i^{D_u},d_k^{D_u})} \ge \left(\frac{2}{3}\right)^{\alpha_1}\left(p_1 + \frac{2}{3}q_1\right)$, where $p_1 + q_1 = n(n-1)$, $\alpha = \left\lfloor \frac{|u|(n-l)}{n-1} \right\rfloor$ and $p_1\alpha_1 + q_1(\alpha_1 + 1) = n|u|(n-l)$. Similarly, we can prove the last sum term in (14), which completes the proof.

Corollary 1. *For any two-level combined design $D_c^w \in \mathcal{C}(n, 2^s)$ and $1 \le k \le s$, we have $[I_k(D_c^w)]^2 \ge \sum_{|u|=k} LB_{1u}$ where LB_{1u} is defined in (13).*

Example 2. Consider the following design $D \in \mathcal{D}(4; 2^7)$ and the two foldover plans γ_1 and γ_2.

Design	D						
	0	0	0	1	1	1	1
	1	0	1	1	0	0	0
	1	1	0	0	1	1	0
	0	1	1	0	0	0	1
γ_1	1	0	1	0	1	1	0
γ_2	1	1	1	0	0	1	0

The corresponding projection discrepancy and their lower bounds as well as the UP of the original design D and the combined designs D^w_{c1} and D^w_{c2} for the foldover plans γ_1 and γ_2 are shown as follows.

k		1	2	3	4	5	6	7
$MI_k(D)$		0	0.0781	0.2676	0.3655	0.2490	0.0847	0.0115
LB_{1u}		0.2188	0.7072	1.1068	0.9895	0.4950	0.1299	0.0149
γ_1	$I_k(D^w_{c1})$	0.2188	0.8634	1.4291	1.2688	0.6369	0.1713	0.0193
	$MI_k(D^w_{c1})$	0	0.0625	0.2070	0.2742	0.1815	0.0601	0.0080
γ_2	$I_k(D^w_{c2})$	0.2188	0.8166	1.2826	1.0861	0.5233	0.1361	0.0149
	$MI_k(D^w_{c2})$	0	0.0156	0.0605	0.0916	0.0680	0.0249	0.0036

Observe that $MI_k(D^w_{c2}) < MI_k(D^w_{c1}) < MI_k(D)$, for $1 < k \leq 7$ and $I_k(D^w_{c1}) \geq I_k(D^w_{c2}) \geq LB_{1u}$, for $k \leq 7$. Hence D^w_{c2} has better projection uniformity than D^w_{c1} and both of them are better than D under MD. Further, γ_2 is better than γ_1.

4. Projection uniformity for general follow-up designs

In foldover designs, the additional number of runs should be equal to the original design. This requirement can be relaxed by adding any number of runs in the follow-up step, and the resulting designs are called follow-up designs. In this section, we discuss the projection discrepancy and related properties for two-level follow-up design as a generalization of Section 3.

Let V_s be the set of all $v_s(=2^s)$ level combinations arranged in the lexicographical order. For a design $D \in \mathcal{D}(n, 2^s)$, let $n(i_1, \ldots, i_s)$ denote the number of times that the point $(i_1, \ldots, i_s)$ occurs in D and $\boldsymbol{y}_D$ be the $v_s \times 1$ vector with elements $n(i_1, \ldots, i_s)$ arranged in the lexicographical order. Define $A = \begin{pmatrix} 7/6 & 1 \\ 1 & 7/6 \end{pmatrix}$, $M_s = \bigotimes_{i=1}^{s} A$, where $\bigotimes$ is the Kronecker product. Then for any design $D \in \mathcal{D}(n, 2^s)$, the expression of $[MD(D)]^2$ can be rewritten as (see Chen et al., 2015)

$$[MD(D)]^2 = \left(\frac{19}{12}\right)^s - 2\left(\frac{305}{192}\right)^s + \frac{1}{n^2}\left(\frac{3}{2}\right)^s \boldsymbol{y}'_D M_s \boldsymbol{y}_D. \tag{15}$$

Let $\mathcal{D}_{0s}(N, 2^s)$ be a class of two-level, N-run and s-factor U-type designs. Denote $\mathcal{D}_{1s}(n, 2^s)$ as a class of two-level, n-run and s-factor designs where the levels of each factor differ by at most one. Hence, N must be an even integer and n could be any integer. We use D_{0s} and D_{1s} to represent the designs of initial experiment and second-step experiment, respectively. Denote all of the follow-up designs $D^E_s = (D'_{0s}, D'_{1s})'$ as $\mathcal{D}^E_s(N+n, 2^s)$, and D^E_u, D_{0u} and D_{1u} are the projection of D^E_s, D_{0s} and D_{1s} on C^u, respectively. Then, $D^E_u = (D'_{0u}, D'_{1u})'$ and $\boldsymbol{y}_{D^E_u} = \boldsymbol{y}_{D_{0u}} + \boldsymbol{y}_{D_{1u}}$.

According to (15), the squared mixture discrepancy value of D^E_u can be rewritten as

$$\begin{aligned}[MD(D^E_u)]^2 &= \left(\frac{19}{12}\right)^{|u|} - 2\left(\frac{305}{192}\right)^{|u|} + \frac{1}{(N+n)^2}\left(\frac{3}{2}\right)^{|u|} \boldsymbol{y}'_{D^E_u} M_u \boldsymbol{y}_{D^E_u} \\ &= \frac{2Nn}{(N+n)^2}\Delta_u + \frac{N^2}{(N+n)^2}[MD(D_{0u})]^2 + \frac{n^2}{(N+n)^2}[MD(D_{1u})]^2 + \left(\frac{3}{2}\right)^{|u|} \frac{2}{(N+n)^2} \boldsymbol{y}'_{D_{0u}} M_u \boldsymbol{y}_{D_{1u}},\end{aligned} \tag{16}$$

where $\Delta_u = \left(\frac{19}{12}\right)^{|u|} - 2\left(\frac{305}{192}\right)^{|u|}$.

Next, we consider the lower bound of projection discrepancy for follow-up designs. Based on the expression of MD, Zhou et al. (2013) proposed a lower bound for any two-level design as follows.

Lemma 3. *For any design $D \in \mathcal{D}(n, 2^s)$, we have*

$$[MD(D)]^2 \geq \left(\frac{19}{12}\right)^s - 2\left(\frac{305}{192}\right)^s + \left(\frac{39}{24}\right)^s + \frac{1}{n^2}\left(\frac{3}{2}\right)^s \sum_{r=1}^{s} \binom{s}{r} \frac{s_{n,r,2}}{6^r}\left(1 - \frac{s_{n,r,2}}{2^r}\right),$$

and $s_{n,r,2}$ is the remainder at division of n by 2^r.

Following Lemma 3, denote $LB([MD(D_{0u})]^2)$ and $LB([MD(D_{1u})]^2)$ as the corresponding lower bounds of the MD-values of the projected initial experiment and second-step experiment, respectively. Then from Lemma 3, Eq. (16) and Lemma 4 in Gou et al. (2018), we can obtain the following lower bound of MD-value for the projected follow-up designs.

Proposition 1. *For any design $D_u^E \in \mathcal{D}_u^E(N+n, 2^{|u|})$, we have $[MD(D_u^E)]^2 \geq LB_{2u}$, where*

$$LB_{2u} = \frac{2Nn}{(N+n)^2}\Delta_u + \frac{N^2}{(N+n)^2}LB([MD(D_{0u})]^2) + \frac{n^2}{(N+n)^2}LB([MD(D_{1u})]^2) + \left(\frac{3}{2}\right)^{|u|}\frac{2}{(N+n)^2}B\left(\frac{7}{6}\right),$$

and $B(\delta) = p\delta^w + q\delta^{w+1}$, w is the largest integer contained in $|u|/2$, p and q are nonnegative integers satisfying $p+q = Nn$ and $pw + q(w+1) = Nn|u|/2$.

Moreover, from Lemma 3, Eq. (16) and Lemma 5 in Gou et al. (2018), we can obtain another lower bound of MD-value for the projected follow-up designs as follows.

Proposition 2. *For any design $D_u^E \in \mathcal{D}_u^E(N+n, 2^{|u|})$ and D_{0u} is an $OA(N, |u|, t)$, we have $[MD(D_u^E)]^2 \geq LB_{3u}$, where*

$$LB_{3u} = \frac{2Nn}{(N+n)^2}\Delta_u + \frac{N^2}{(N+n)^2}LB([MD(D_{0u})]^2) + \frac{n^2}{(N+n)^2}LB([MD(D_{1u})]^2) + \left(\frac{3}{2}\right)^{|u|}\frac{2n}{(N+n)^2}\sum_{j=0}^{t}\left(\frac{1}{6}\right)^j\binom{|u|}{j}v_j,$$

and v_j is the largest integer below $N/2^j$.

Combining Proposition 1 with Proposition 2, we can obtain the following result.

Theorem 5. *For any design $D_u^E \in \mathcal{D}_u^E(N+n, 2^{|u|})$, we have $[MD(D_u^E)]^2 \geq LB_{4u}$, where $LB_{4u} = \max\{LB_{2u}, LB_{3u}\}$.*

It is to be remarked that since we have already experimented the design D_{0u}, we can replace $LB([MD(D_{0u})]^2)$, by its actual value $[MD(D_{0u})]^2$. And redefining the projection discrepancy as $[I_k(D_s^E)]^2 = \sum_{|u|=k}[MD(D_u^E)]^2/\binom{s}{k}$ here, we can also get the lower bound of $[I_k(D_s^E)]^2$ as follows.

Corollary 2. *For any design $D_s^E \in \mathcal{D}_s^E(N+n, 2^s)$ and $1 \leq k \leq s$, we have $I_k(D_s^E) \geq \sum_{|u|=k}LB_{4u}/\binom{s}{k}$, where LB_{4u} is defined in Theorem 5.*

With the lower bound of projection discrepancy which can be a benchmark, one can more efficiently and systematically find designs with good projection uniformity by some useful algorithm.

5. Uniformity pattern for three-level designs under MD

In this section, we define the UP for three-level designs and give more statistical justification of UP and MPU under MD. For the three-level factorials, we consider all the level permutations and discuss the average projection discrepancy as UP and obtain the relationship with GWP.

For any $D \in \mathcal{D}(n, 3^s)$, when considering all 3! possible level permutations for every factor, we can obtain $(3!)^s$ isomorphic designs. We denote the set of these designs by $\mathcal{P}(D)$. Because reordering the rows or columns does not change the geometrical structure and statistical properties of a design, we do not consider this situation here. All designs in $\mathcal{P}(D)$ share the same GWP, but may have different projection discrepancies. In this part, we compute the average projection discrepancy value of all designs in $\mathcal{P}(D_u)$ as UP and show the relationship with GWP. Thus, for $1 \leq K \leq s$ and $|u| = K$, we define

$$\bar{I}_K(D) = \frac{1}{(3!)^K}\sum_{D'_u \in \mathcal{P}(D_u)}[I_K(D')]^2 = \frac{1}{(3!)^K}\sum_{D'_u \in \mathcal{P}(D_u)}\sum_{|u|=K}[MD_u(D')]^2.$$

Similarly, we define the MPU criteria as that in (9) by substituting $MI_k(D)$ with $\bar{I}_K(D)$. According to formula (2) and (3), for any $D \in \mathcal{D}(n, 3^s)$, it is shown that

$$[MD_u(D)]^2 = \left(\frac{7}{12}\right)^K - \frac{2}{n}\sum_{i=1}^{n}\prod_{j\in u}f_1(x_{ij}) + \frac{1}{n^2}\sum_{i,k=1}^{n}\prod_{j\in u}f(x_{ij}, x_{kj}),$$

where $f(x_{ij}, x_{kj}) = k_j(x_{ij}, x_{kj})$ in (1) and $f_1(x_{ij}) = \int_{[0,1)}k_j(x_{ij}, y)dy = \frac{2}{3} - \frac{1}{4}|x_{ij} - \frac{1}{2}| - \frac{1}{4}|x_{ij} - \frac{1}{2}|^2$.

As similar as the result in Section 3 of Zhou and Xu (2014), we can obtain that

$$\frac{2}{n}\sum_{|u|=K}\sum_{D'_u\in\mathcal{P}(D_u)}\sum_{i=1}^{n}\prod_{j\in u}f_1(x_{ij})=\frac{2}{n}\sum_{|u|=K}n\left(2!\sum_{p=0}^{2}f_1\left(\frac{2p+1}{6}\right)\right)^K$$

$$\frac{1}{n^2}\sum_{|u|=K}\sum_{D'_u\in\mathcal{P}(D_u)}\sum_{i,k=1}^{n}\prod_{j\in u}f(x_{ij},x_{kj})=\frac{1}{n^2}\sum_{|u|=K}(3!)^K\left(\frac{c_1}{6}\right)^K\sum_{i,k=1}^{n}c_2^{\delta_{ik}},$$

where $c_1=\sum_{p=0}^{2}\sum_{p\neq l}f\left(\frac{2p+1}{6},\frac{2l+1}{6}\right)=\frac{13}{4}, c_2=2\sum_{p=0}^{2}f\left(\frac{2p+1}{6},\frac{2p+1}{6}\right)/c_1=\frac{55}{39}$ and δ_{ik} denotes the number of places where they take the same value for two rows $\boldsymbol{x}_i$ and $\boldsymbol{x}_k$ of any design D_u. Because $f(\cdot,\cdot)$ satisfies the condition of Lemma 1 of Zhou and Xu (2014) (that is, $f(x,y)\geq 0$ and $f(x,x)+f(y,y)\geq f(x,y)+f(y,x)$ for any $x\neq y, x,y\in[0,1]$) and $c_2>1$, according to the lemmas in the Appendix of Zhou and Xu (2014) we can obtain that

$$\sum_{i,k=1}^{n}c_2^{\delta_{ik}}=n^2\left(\frac{c_2+2}{3}\right)^K\sum_{v=0}^{K}\left(\frac{c_2-1}{c_2+2}\right)^v A_v\left(D_u\right).$$

Thus, after simplification we can obtain the following result.

Theorem 6. *For any design $D\in\mathcal{D}(n,3^s)$, we have*

$$\bar{I}_K(D)=\binom{s}{K}\left(\frac{7}{12}\right)^K-2\binom{s}{K}\left(\frac{16}{27}\right)^K+\left(\frac{133}{216}\right)^K\sum_{v=0}^{K}\left(\frac{16}{133}\right)^v\binom{s-v}{s-K}A_v\left(D\right).$$

Clearly, the average projection discrepancy is a linear combination of GWP under all level permutations under MD. And we can generate designs with smaller projection discrepancy values than the average value by permuting levels of the projected design from Theorem 6.

6. Conclusion

In this paper, we discuss the projection uniformity and related properties under MD. The UP is defined under MD for two-level designs and the linear relationship between UP and GWP is obtained. Under MD, the uniformity resolution and MPU of the two-level fraction factorial designs are almost equivalent to resolution and GMA, respectively. Furthermore, it is shown that foldover strategy can improve the uniformity resolution. For general follow-up designs, the projection discrepancy and the corresponding lower bound are also given. Moreover, we use the average projection discrepancy to define the UP for three-level designs based on level permutations and show that the average projection discrepancy is also a linear combination of GWP when considering all level permutations under MD.

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