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TWO-LEVEL ISOMORPHIC FOLDOVERS DESIGNS

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Abstract: Two-level orthogonal arrays ensure the independent estimations of main effects when linear models are considered, and thus are popularly used experimental designs. Such arrays can be classified into regular and nonregular designs (Wu and Hamada, 2021). Regular designs entertain specific algebraic structures and thus have been well studied in the literature. Their run sizes, however, are limited to powers of 2. Nonregular designs have a more complicated structure, but they are more flexible in the run sizes and allow the estimation of more effects. The construction of nonregular designs remains a challenge. This paper introduces a new class of nonregular designs called isomorphic foldovers design (IFD). Specifically, it is composed of several foldovers of an initial design. The goal of our study is to investigate the general theory of IFDs. We propose a method for obtaining all nonequivalent IFDs with f foldovers for any initial design. Two algorithms are provided to construct optimal f-IFD in terms of G-aberration (or G_2-aberration) criterion. The IFD structure provides an efficient way to find good designs in the sense that constructing good IFDs based on a nonregular initial design is often more successful than doing so with a more granular single flat. Meanwhile, the IFDs have a parallel flats structure and thus are much easier to understand and analyze than many other nonregular designs. Moreover, we show that some existing designs can be viewed as special cases of IFDs.

Key words and phrases: Foldover, G-aberration criterion, nonregular design, screening experiment.

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1. Introduction

Two-level orthogonal arrays can be roughly classified into regular and nonregular designs according to the aliasing structure (Wu and Hamada, 2021). The estimated effects of a regular design are either orthogonal or fully aliased. Their run sizes are limited to a power of 2. Two-level regular designs have been well studied and enumerated, see e.g. Box and Hunter (1961), Draper and Mitchell (1967), Chen and Lin (1991), Chen et al. (1993), Mee (2009), Xu (2009), Shrivastava and Ding (2010), Liu et al. (2011), Wu and Hamada (2021) and the reference therein. In contrast, the estimated effects in a nonregular design can be partially confounded. Compared with regular designs, nonregular designs have a more complicated aliasing structure, but they have more flexible run sizes (a multiple of 4). In addition, nonregular designs allow for estimating more effects.

While nonregular designs have many advantages, their construction method remains a challenge. Most construction methods for nonregular designs in the literature are restricted to some specific number of runs. For example, Sun (1993) enumerated all nonisomorphic nonregular designs with 16 runs and up to 14 factors. Connor and Young (1961) proposed parallel flats designs (PFDs). A PFD with f flats (f-PFD) consists of f 2^{k-p} designs in which the fractions are determined by the same p defining words but different sign assignments. PFDs are a class of nonregular designs that retain some of the simplicity of regular designs. They enjoy many desirable properties and thus have received widespread attention, see Wang and Mee (2021) for a comprehensive review of PFDs. Xu (2005) and Xu and Wong (2007) constructed nonregular designs

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from codes. Their run sizes, however, are limited to a power of 2. Mee (2009, Section 6.3) gave a useful summary of strength 2 designs with up to 48 runs; also see Sections 7.3 and 8.2 for nonregular designs with higher strength. Schoen et al. (2010) specified an algorithm to enumerate a minimum complete set of combinatorially non-isomorphic orthogonal arrays. Doković et al. (2014) and Shi and Tang (2018) studied nonregular designs from Hadamard matrices. Vazquez et al. (2019) constructed strength-three designs with 64 and 128 runs by concatenating two designs via an effective column change/variable neighborhood search algorithm. Vazquez et al. (2022) extended this method for constructing strength-three designs with 80, 96 and 112 runs. Vazquez and Xu (2019) constructed a class of strength-three nonregular designs, while Wang and Mee (2021) and Edwards and Mee (2023) constructed low G-aberration PFDs. These nonregular designs are composed of several isomorphic copies of the initial regular design. They enjoy a simple structure and desirable properties. The run sizes of the initial designs, however, are limited to powers of 2.

Here we introduce a new class of nonregular designs, called isomorphic foldovers designs (IFDs). An IFD with f foldovers (f-IFD) consists of several foldovers of a given initial design, where the initial design can be either regular or nonregular. Foldover is a classic technique used to create a follow-up experiment. All foldover designs are obtained by reversing the sign of columns of the initial design. For more development on foldover designs, we refer to Webb (1968), Montgomery and Runger (1996), Cheng (1998), Li and Mee (2002), Fang et al. (2003), Li and Lin (2003), Li et al. (2003), Cheng et al. (2008) and Elsawah and Qin (2015). When the initial design is regular, a

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f-IFD degenerates into an f-PFD. Moreover, since any initial design can be expressed as a g-PFD, every f-IFD is essentially a (gf)-PFD for some $g \leq n$. That is, IFDs are subsumed within PFDs. Most importantly, it will be shown that constructing good IFDs based on a nonregular initial design is often more successful than doing so with a more granular single flat.

This paper aims to study the general theory of IFDs. For any given initial design, we propose a method for obtaining all nonequivalent f-IFDs for any $f \geq 2$. Two algorithms are provided to construct the optimal f-IFD in terms of G-aberration (or G_2-aberration) criterion. These algorithms are feasible and straightforward to implement. The IFD structure provides an efficient way to find good designs. At the same time, the IFDs can be characterized as PFDs and thus are much easier to understand and analyze than many other nonregular designs (Edwards and Mee, 2023). Moreover, we show that IFDs include several existing designs as special cases.

This paper is organized as follows. Section 2 introduces the notation and preliminaries. Section 3 proposes the theoretical results of f-IFDs. A method for obtaining all nonequivalent f-IFDs is proposed for any given initial design. Two algorithms are developed in Section 4 to construct optimal f-IFDs in terms of G-aberration (or G_2-aberration) criterion. Concluding remarks and discussion are provided in Section 5. All proofs are deferred to the Supplementary Material.

2. Definitions and preliminaries

Let D be a two-level orthogonal array with N runs and k factors, where each row indicates a treatment combination and each column represents a factor with levels ± 1.

There are in total of 2^k possible treatment combinations for k factors. We call the set of these 2^k runs a design space for k factors, denoted as $\mathcal{A}$. Then design D can be seen as a collection of runs in $\mathcal{A}$. Following Fontana et al. (2000), Ye (2003) and Butler (2008), the indicator function of D is a function defined on $\mathcal{A}$ such that $F(x) = f_x$, where f_x is the frequency of run $x = (x_1, \ldots, x_k)$ for $x \in \mathcal{A}$. For a unreplicated design D, $F(x) = 0$ or 1 for any $x \in \mathcal{A}$. Let $X_V(x) = \prod_{v \in V} x_v$ on $\mathcal{A}$ for $V \in \mathcal{P}$, where $\mathcal{P}$ is the collection of all subset of $\{1, \ldots, k\}$. Then the indicator function of D has the following polynomial form

$$F(x) = \sum_{V \in \mathcal{P}} b_V X_V(x),$$

where $b_V = 1/2^k \sum_{x \in D} X_V(x)$ for $V \in \mathcal{P}$. In particular, $b_\emptyset = N/2^k$. For $V = \{v_1, \ldots, v_q\}$, an index of q columns of D, the J_q-characteristic is defined as $J_q(V) = |\sum_{x \in D} X_V(x)|$. If $J_q(V) = N$, the corresponding q columns of D form a complete word. If $0 < J_q(V) < N$, the corresponding q columns form a partial word. Obviously, the complete word indicates full aliasing among associated factorial effects, while the partial word represents partial aliasing among them. Following Li et al. (2003), $\rho(V) = J_q(V)/N$ measures the aliasing degree of the word $X_V(x)$ with the intercept. In the remainder of the paper, we call $\rho(V)$ the aliasing index of $X_V(x)$ as that in Cheng et al. (2004). The aliasing index for regular designs is either 0 or 1. For the nonregular design, there is at least one aliasing index whose value is between 0 and 1. Following Deng and Tang (1999), the confounding frequency vector (CFV) of design D is defined as

$$\text{CFV}(D) = [(f_{11}, \ldots, f_{1N})_1, \ldots, (f_{k1}, \ldots, f_{kN})_k],$$

where f_{qj} denotes the frequency of the words with aliasing index $(N + 1 - j)/N$ for

$q = 1, \ldots, k$ and $j = 1, \ldots, N$. Let r be the smallest integer such that $\max_{|V|=r} \rho(V) > 0$, where $|V|$ denotes the cardinality of set V. The generalized resolution (GR) (Deng and Tang, 1999) is defined as

$$\mathrm{GR}(D) = r + 1 - \max_{|V|=r} \rho(V).$$

The G-aberration criterion is then proposed (Deng and Tang, 1999) to sequentially minimize the components in the confounding frequency vector from left to right. That is, if two designs have $f_{q^*j^*}$ as the first nonequal component in their confounding frequency vectors, the design with smaller $f_{q^*j^*}$ is preferred in terms of G-aberration criterion, and we say it has less G-aberration. A design is called the minimum G-aberration design if there is no other design with the same size has a less G-aberration.

Tang and Deng (1999) proposed G_2-aberration criterion, which is a relaxed version of G-aberration criterion. For $q = 1, \ldots, n$, define $B_q(D) = \Sigma_{|V|=q}(\rho(V))^2$. Design D's generalized wordlength pattern is $\mathrm{GWLP}(D) = [B_1(D), \ldots, B_n(D)]$. Similar to the G-aberration criterion, the G_2-aberration criterion sequentially minimizes the components of the generalized wordlength pattern from left to right. Following Hedayat et al. (1999), two two-level designs are called isomorphic if one of them can be obtained from the other one by row permutations, column permutations, and sign switches of columns. Two isomorphic designs have the same confounding frequency vector, while the reverse is not true, see Chen and Lin (1991). For regular designs, both the confounding frequency vector and generalized wordlength pattern degenerate to the wordlength pattern, and thus both the minimum G-aberration criterion and minimum G_2-aberration criterion degenerate to the minimum aberration criterion.

Example 1. Given $N = 16$ and $k = 10$, Sun (1993) shows that there are 78 nonisomorphic 16×10 designs, denoted as $10.z$ for $z = 1, \ldots, 78$. The 78 nonisomorphic designs can also be found in Schoen et al. (2010). The minimum aberration regular 2^{10-6} design 10.4, has generators

$$x_3 = x_1x_2, x_5 = x_1x_4, x_6 = x_2x_4, x_7 = x_1x_8, x_9 = x_1x_2x_4x_8, \text{and } x_t = x_2x_4x_8,$$

where $t = 10$. The indicator function is

$$\begin{aligned} F(x_1, \ldots, x_t) &= \frac{1}{2^6}(1 + x_1x_2x_3)(1 + x_1x_4x_5)\cdots(1 + x_6x_7x_9) \\ &= \frac{1}{64} + \frac{1}{64}x_1x_4x_5 + \frac{1}{64}x_1x_2x_3 + \frac{1}{64}x_2x_3x_4x_5 + \cdots + \frac{1}{64}x_3x_5x_8x_t. \end{aligned}$$

It has 63 terms (besides the constant), corresponding to the defining words. It has CFV=$[(8,0)_3, (18,0)_4, (16,0)_5, (8,0)_6, (8,0)_7, (5,0)_8]$ and GR=3. Next, consider the minimum G-aberration nonregular design 10.48. The indicator function is

$$F(x_1, \ldots, x_t) = \frac{1}{2^{10}}(16 + 8x_1x_5x_7 + 8x_1x_5x_8 + \cdots + 16x_3x_4x_5x_6x_7x_8x_9x_t),$$

where the complete formula can be found in the Supplementary Material. There are 207 items (besides the constant), of which 15 terms have a coefficient of $\frac{16}{2^{10}}$ and the remaining 192 terms have a coefficient of $\frac{8}{2^{10}}$, corresponding to 15 complete words and 192 partial words of aliasing index 1/2 respectively. It has CFV=$[(0,32)_3, (10,32)_4, (0,64)_5,$ $(0,32)_6, (0,32)_7, (5,0)_8]$ and GR=3.5. Design 10.48 has less G-aberration and a larger generalized resolution than design 10.4.

For a $n \times k$ design D_0, denote a foldover plan by a $1 \times k$ row vector γ, in which each element represents whether the corresponding factor is reversed. For example, foldover plan $\gamma = (0, \ldots, 0)$ indicates no factor's sign is reserved. We call this type of foldover plan a no-factor foldover plan and the corresponding foldover design a no-factor foldover. Foldover plan $\gamma = (1, \ldots, 1)$ indicates that the signs of all factors are reserved. We call this type of foldover plan an all-factor foldover plan and the corresponding foldover design an all-factor foldover.

Definition 1. Let D_0 be a design with n runs and k factors, then there are 2^k possible options for the foldover vector γ, corresponding to 2^k foldovers of D_0. The row concatenation of any f distinct foldovers is called an isomorphic foldovers design with f foldovers (f-IFD).

It is clear that all possible 2^k foldovers form the full 2^k design (with n repetitions), while any two distinct foldovers must be isomorphic. The f-IFD can be defined by an $f \times k$ matrix, which is called the foldover matrix of the f-IFD,

$$\Gamma = (\gamma_1^T, \ldots, \gamma_f^T)^T,$$

where $\gamma_i = (\gamma_{i1}, \ldots, \gamma_{ik})$ is the foldover plan of the ith foldover. Then we have the following result.

Lemma 1. *Let* $F_0(x) = \sum_{V \in \mathcal{P}} b_V X_V(x)$ *be the indicator function of the initial design* D_0*, then the* f*-IFD defined by foldover matrix* Γ*, say* D*, has the indicator function*

$$F(x) = \sum_{V \in \mathcal{P}} \sum_{i=1}^{f} (-1)^{\prod_{v \in V} \gamma_{iv}} b_V X_V(x).$$

From Lemma 1, the word $X_V(x)$, with aliasing index $\rho(V)$ in D_0, has aliasing index

$$[\rho(V)/f] \left| \sum_{i=1}^{f} (-1)^{\prod_{v \in V} \gamma_{iv}} \right|$$

in D. Then we are ready to propose the following result.

Lemma 2. *Let D be an f-IFD based on the initial design D_0, then D has the same or fewer words than D_0. For any common word of D and D_0, it has the same or smaller aliasing index as a word in D than that in D_0. Particularly, if D_0 does not have a complete word, then neither does D. For the case of $f = 2$, any word of D_0 either is removed or keeps the aliasing index unchanged in D.*

For even $f > 2$, an f-IFD can sometimes be reduced, in the sense that it is an $f/2$-IFD composed of foldovers of size $2n$. The following result gives insights into understanding the structure of IFDs with an even number of foldovers.

Theorem 1. *Consider an f-IFD defined by foldover matrix Γ, where $\Gamma = (\gamma_{ij})$ is an $f \times k$ matrix for even $f > 2$. Suppose the rows of Γ can be paired so that the product of the two rows of each pair is identical. Then the f-IFD can be reduced into an $f/2$-IFD with the foldover matrix $\hat{\Gamma} = (\hat{\gamma}_{ij})$, therein $\hat{\Gamma}$ is of size $f/2 \times k$ and*

$$\hat{\gamma}_{ij} = \begin{cases} 1 & i = 1,\ j = 1, \ldots, k, \\ \gamma_{(2i-1)j}\gamma_{1j} & i = 2, \ldots, f/2,\ j = 1, \ldots, k. \end{cases}$$

Example 2. Given $k = 7, f = 6$, let D be the 6-IFD defined by foldover matrix

$$\Gamma = (\gamma_1^T, \ldots, \gamma_f^T)^T = \begin{bmatrix} 1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & -1 & 1 & -1 & 1 \\ -1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & -1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 \end{bmatrix}.$$

It is easily checked that $\gamma_1\gamma_2 = \gamma_3\gamma_4 = \gamma_5\gamma_6$. Then each of the two 2×7 matrices $(\gamma_3^T, \gamma_4^T)^T$ and $(\gamma_5^T, \gamma_6^T)^T$ can be obtained from $(\gamma_1^T, \gamma_2^T)^T$ by sign switches of columns, indicating that these two matrices correspond to two foldovers of the 2-IFD defined by the foldover matrix $(\gamma_1^T, \gamma_2^T)^T$. That is, D is a 6-IFD given by a $n \times 7$ design D_0, and the 6-IFD can be reduced into a 3-IFD, where D_0 is now a $2n \times 7$ design given by the 2-IFD obtained from the foldover matrix $(\gamma_1^T, \gamma_2^T)^T$.

3. General properties of f-IFDs

For any two-level orthogonal array with n runs and k factors D_0, let W be the set of its e words and $\{w_1, \ldots, w_u\}$ be the basic words of D_0. That is, all e words can be generated by the u words in $\{w_1, \ldots, w_u\}$. Obviously, we have $u \leq k$ and $e \leq 2^u - 1$. It is clear that $u = k - \log_2 n$ and $e = 2^u - 1$ for regular D_0. Without loss of generality, suppose the words in W are arranged in Yates order. Note that $\{w_1, \ldots, w_u\}$ can generate $2^u - 1$ words, while not all these words appear in W when $e < 2^u - 1$.

Example 3. Revisit designs 10.4 and 10.48 in Example 1. Design 10.4 is a regular 2^{10-6} design with 63 complete words generated by 6 basic words $\{x_1x_2x_3, x_1x_4x_5, x_1x_7x_8, x_1x_9x_t, x_2x_4x_6, x_6x_7x_9\}$. Here we have $u = 6$ and $e = 2^u - 1 = 63$ for design 10.4. Design 10.48 has 15 complete words and 192 partial words of aliasing index 1/2. It can be easily confirmed that design 10.48 is an 8-PFD. The single flat is a 2^{10-9} design with 511 complete words generated by $X = \{x_1x_5x_7, x_1x_5x_8, x_1x_5x_9, x_1x_5x_t, x_1x_6x_7, x_2x_5x_7, x_3x_5x_9, x_3x_7x_9, x_4x_5x_9\}$. Among the 511 complete words of the single flat, 192 words become partial words of aliasing index 1/2, 15 words remain complete words and the remaining 304 words are removed in design 10.48. It is clear that all 207 words of design 10.48

can be generated by the 9 words in X. Thus, we have $u = 9$ and $e = 207$ for design 10.48.

Lemma 3. *Let D_0 be a design with n runs, k factors and e words. Then D_0 has $u = k - \log_2(n/g)$ basic words with $e \leq 2^u - 1$, where g is the number of flats of D_0 when it is characterized as a parallel flats design. In particular, if D_0 is regular, then $u = k - \log_2 n$ and $e = 2^u - 1$; and if D_0 is a n-PFD, then $u = k$.*

From Lemma 3, the basic words of design D_0 can be easily obtained from its single flat instead of a comprehensive examination. Example 3 well illustrates this issue. Another illustrative example of the 12-run Plackett-Burman design is deferred to the Appendix.

For design D_0, each of the 2^k foldovers corresponds to a column of a Sylvester Hadamard matrix of order 2^u. We next describe this connection. Let H_{2^u} be a Sylvester Hadamard matrix of order 2^u, generated by the recursion

$$H_{2^1} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \text{and } H_{2^i} = \begin{bmatrix} H_{2^{i-1}} & H_{2^{i-1}} \\ H_{2^{i-1}} & -H_{2^{i-1}} \end{bmatrix} \text{ for } i \geq 2.$$

H_{2^u} is symmetrical and $H_{2^u}^2 = 2^u E_{2^u}$, where E_{2^u} represents the identity matrix of order 2^u. We number the columns of H_{2^u} beginning with h_0. Then we have

$$H_{2^u} = [h_0, h_1, \ldots, h_{2^u - 1}].$$

Therein h_0 is the $2^u \times 1$ column vector with all elements unity, and columns $\{h_1, h_2, \ldots, h_{2^{u-1}}\}$ are u basic columns. Any other columns can be generated by them, such as $h_3 = h_1 h_2$, where $ab = (a_1 b_1, \ldots, a_z b_z)^T$ for any $a = (a_1, \ldots, a_z)^T$ and $b = (b_1, \ldots, b_z)^T$.

Each of the 2^k foldovers corresponds to a column of H_{2^u}, in that h_i determines the sign switch of each basic word in the ith foldover relative to D_0. Note that every 2^{k-u} foldover corresponds to the same column of H_{2^u}, and which one of these foldovers to choose has no effect on the indicator function of the resulting f-IFD. Thus, instead of choosing f foldovers from 2^k foldovers, we need only choose f foldovers from 2^u foldovers that correspond to H_{2^u} to obtain all possible relevant f-IFDs. Without loss of generality, assume that the signs of the first $k-u$ factors that can not be generated by the words $\{w_1, \ldots, w_u\}$ keep unchanged in each of the f foldovers. In this way, to obtain an f-IFD, we choose f foldovers from 2^u foldovers, that is, we choose f columns from H_{2^u}. By restricting our attention to unreplicated designs, there are $2^u!/\{f!(2^u-f)!\}$ combinations to be considered.

Without loss of generality, we take the first foldover to be the no-factor foldover, that is, the column h_0. Each of the remaining isomorphic foldovers corresponds to a column of $H^* = [h_1, \ldots, h_{2^u-1}]$. Thus the number of combinations is reduced to $(2^u-1)!/\{(f-1)!(2^u-f)!\}$. Some of these combinations will produce equivalent f-IFDs, with the following definition.

Definition 2. Two f-IFDs are called equivalent if one f-IFD can be obtained from the other by row permutations and column sign switches.

It is clear that two equivalent f-IFDs must be isomorphic while the reverse is not true. For a subset of $f-1$ columns of H^*, say $z = \{h_{c_1}, \ldots, h_{c_{f-1}}\}$, let $\tilde{z} = \{h_0, z\}$, which indicates including the no-factor foldover D_0. It is easy to see that $\tilde{z}$ is determined by the $u \times f$ matrix consisting of the rows with index $\{1, 2, 4, \ldots, 2^{u-1}\}$ of $\tilde{z}$, and we call it the B matrix of this f-IFD. Thus we have the following result.

Theorem 2. *The f-IFD corresponding to $\tilde{z}$ has the foldover matrix $\Gamma = (\gamma_{i,j})_{f\times k}$ with*

$$\begin{cases} \prod_{v\in w_l} \gamma_{iv} = b_{li} & i = 1,\dots,f, l = 1,\dots,u, \\ \gamma_{iv} = 1 & i = 1,\dots,f, v \in F_0, \end{cases}$$

where $\{w_1,\dots,w_u\}$ are the basic words of D_0, b_{li} represents the (l,i) element of B for $l = 1,\dots,u$, $i = 1,\dots,f$, and F_0 consists of the first $k-u$ factors of D_0 that can not be generated by its basic words.

Theorem 2 illustrates the relationship between the foldover matrix and B matrix of an f-IFD. It can be easily verified that the u factors not in F_0 can be generated by the u words $\{w_1,\dots,w_u\}$. Combining these with Theorem 1, we have the following result.

Corollary 1. *For an f-IFD based on B with even $f > 2$, if the columns of B can be paired so that the product of the two columns of each pair is identical, then the f-IFD can be reduced into an $f/2$-IFD.*

Following Wang and Mee (2021), let the group of $\tilde{z} = \{h_0, z\}$, where z is subset of $f-1$ columns of H^*, be

$$G_{\tilde{z}} = \{h_{c_j}\cdot\tilde{z} : j = 0,1,\dots,f-1\}, \text{ with } h_{c_j}\cdot\tilde{z} = \{h_{c_j}, h_{c_j}h_{c_1},\dots,h_{c_j}h_{c_{f-1}}\},$$

where $c_0 = 0$. Then the following result provides a basis to identify equivalent IFDs.

Corollary 2. *For any initial design, two f-IFDs based on different foldovers, $\tilde{z}_1 = \{h_0, z_1\}$ and $\tilde{z}_2 = \{h_0, z_2\}$, are equivalent if and only if $\tilde{z}_1$ and $\tilde{z}_2$ belong to the same group.*

For given u and p, denote the number of disjoint groups as $g_{u,f}$. All nonequivalent IFDs can be obtained by selecting just one from each of the $g_{u,f}$ groups. The following results in Propositions 1 and 2 on grouping are taken from Wang and Mee (2021) and are useful in the paper.

Proposition 1. *For odd f, the size of $G_{\tilde{z}}$ is f. For even $f = \lambda 2^\nu$, where $\lambda, u \geq 1$ and λ is odd, the size of $C_{\tilde{z}}$ might be $\lambda, 2\lambda, \ldots, \lambda 2^\nu$.*

Moreover, the group size indicates the reduction of the f-IFDs. If the size of one group is m with $m < f$, then any f-IDF generated from this group can be reduced into an m-IDF. For any (u, f), let τ_{κ_i} be the frequency of the groups of size κ_i; then the group size pattern (GSP) is defined as $\mathrm{GSP}(u, f) = (\tau_{\kappa_1}, \ldots, \tau_{\kappa_\varsigma})$, with ς different group sizes.

Proposition 2. *For any $f \leq 2^u$,*

$$GSP(u,f) = \left[\frac{t_{u,f}}{f}\right]_f \text{ for odd } f$$

$$GSP(u,4) = \left[\frac{(2^u-1)(2^u-2)}{6}\right]_1, \left[\frac{(2^u-1)(2^u-2)(2^u-4)}{24}\right]_4$$

$$GSP(u,6) = \left[\frac{(2^u-1)(2^u-2)(2^u-4)}{24}\right]_3, \left[\frac{2^u(2^u-1)(2^u-2)(2^u-4)(2^u-8)}{720}\right]_6$$

$$GSP(u,8) = \left[\frac{(2^u-1)(2^u-2)(2^u-4)}{168}\right]_1, \left[\frac{(2^u-1)(2^u-2)(2^u-4)(2^u-8)}{192}\right]_4, \left[\frac{(2^u-1)(2^u-2)(2^u-4)(2^u-8)(8^u-13*4^u+57*2^u-180)}{40320}\right]_8$$

$$GSP(u,10) = \left[\frac{(2^u-1)(2^u-2)(2^u-4)(2^u-6)(2^u-8)}{1920}\right]_5, \left[\frac{2^u(2^u-1)(2^u-2)(2^u-4)(2^u-8)}{720}\right]_{10}.$$

For example, given $u = 4, f = 3$, there are 105 choices for $\tilde{z} = \{h_0, z\}$ with $z = \{h_{c_1}, h_{c_2}\}$. According to the property of H_{16}, there does not exist $c_1 \neq c_2$, such that $h_{c_1} \cdot \tilde{z} = h_{c_2} \cdot \tilde{z}$. Thus the 105 choices of $\tilde{z}$ can be partitioned into $g_{4,3} = 35$ groups of size 3.

Example 4. As discussed in Example 3, design 10.4 has 63 words generated by six basic words. We now consider 6-IFDs based on design 10.4. Given $u = 6$ and $f = 6$, there are $(63)!/(5)!(58)! = 7028847$ choices for $\tilde{z} = \{h_0, z\}$ with $z = \{h_{c_1}, \ldots, h_{c_5}\}$. From Proposition 2, there are 1176357 groups in total, 9765 of size 3 and 1166592 of size 6. That is, $GSP(6, 6) = [9765_3, 1166592_6]$. Similarly, consider 6-IFDs based on design 10.48, where design 10.48 has 207 words generated by nine basic words. Given $u = 9$ and $f = 6$, there are $(511)!/(5)!(506)! = 2.8471 * 10^{11}$ choices for $\tilde{z}$, which can be partitioned into 5516245 groups of size 3 and $4.7449 * 10^{10}$ groups of size 6. We can see that there are much more choices to consider for obtaining all nonequivalent 6-IFDs based on design 10.48 than design 10.4, even if these two designs are of the same size.

Recall that an f-PFD consists of f regular designs from the same family, where the f fractions are determined by the same defining words but different sign assignments. An f-IFD consists of f foldovers of an initial design, where the initial design can be either regular or nonregular. As discussed in Section 1, every f-IFD is essentially a (gf)-PFD for some $g \leq n$. The more general results are summarized in the following theorem.

Theorem 3. *Let D_0 be a two-level design with n runs and k factors.*

(i) *If D_0 is regular, then any f-IFD based on D_0 is an f-PFD.*

(ii) *If D_0 is a g-IFD, then any f-IFD based on D_0 is a (gf)-IFD.*

(iii) *If D_0 is a g-PFD, then any f-IFD based on D_0 is a (gf)-PFD. In particular, any 2-IFD based on D_0 is a $(2g)$-PFD, and it can be reduced into a g-PFD.*

By Theorem 3, any 2-IFD based on a g-PFD is a g-PFD. Obviously, any 2-IFD based on a regular design is a regular design. On one hand, the IFDs generalize PFDs in the sense that PFDs correspond to the special case of the initial design being regular. On the other hand, since any initial design D_0 can be characterized as a g-PFD, every f-IFD is essentially a (gf)-PFD for some $g \leq n$. Moreover Theorem 3 reveals a potential advantage of IFDs, which is to find a lower G-aberration f-IFD instead of searching for a (gf)-PFD. This is especially useful when f is large, where it becomes computationally infeasible to search for a (gf)-PFD.

4. Construction of optimal f-IFD

As mentioned in Section 2, the G-aberration criterion is a popular criterion for ranking designs. Section 3 proposes a method for obtaining all nonequivalent f-IFDs for any given initial design. In this section, two algorithms are developed to search for the optimal f-IFD in terms of G-aberration criterion: 1) an exhaustive search for the minimum G-aberration f-IFD when it is feasible to obtain all nonequivalent f-IFDs; 2) a short-cut to find a low G-aberration f-IFD by iteratively optimizing a random f-IFD, when it is infeasible to obtain all nonequivalent f-IFDs. Examples are provided to show that constructing good IFDs based on a nonregular initial design is often more successful than doing so with a more granular single flat.

We now illustrate how the f columns of H_{2^u} determine the J-characteristics of the f-IFD and present a method for finding the f-IFD with minimum G-aberration

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for any initial design D_0. For any $\tilde{z} = \{h_0, z\}$, where $\{h_{c_1}, \ldots, h_{c_{f-1}}\}$, define $Z_f(z) = 1_{2^u} + \sum_{j=1}^{f-1} h_{c_j}$ and truncate $Z_f(z)$ at e positions corresponding to the words W of D_0, then obtain an $e \times 1$ vector $Z_f(z)|_W$. According to Lemma 1, if we multiply $|Z_f(z)|_W|$ by the J-characteristics of words W, then we can obtain the J-characteristics of the f-IFD corresponding to $\tilde{z}$. For simplicity, we call $Z_f(z)|_W$ and its absolute value $|Z_f(z)|_W|$ the Z-vector and absolute Z-vector, respectively, of the f-IFD. We now present Algorithm 1 for determining the minimum G-aberration f-IFD based on D_0.

Algorithm 1 (An exhaustive search for the minimum G-aberration f-IFD)**.**

Input: A design with n runs and k factors called D_0, and an integer $f \geq 2$.

Output: The minimum G-aberration f-IFD constructed from D_0.

Step 1. For an initial n-run and k-factor design D_0, let $L = (L_1, \ldots, L_e)$ and $J = (J_1, \ldots, J_e)$ be the lengths and J-characteristics of words W arranged in Yates order, respectively.

Step 2. Determine $|Z_f(z)|_W|$ for a representative $\tilde{z}$ from each of the $g_{u,f}$ equivalent groups. Remove duplicate absolute Z-vectors to obtain an $e \times r_{u,f}$ matrix $Z_{u,f}$ where $r_{u,f}$ is the number of the unique absolute Z-vectors.

Step 3. From $Z_{u,f}$ and design D_0's L, we obtain the confounding frequency vectors of all $g_{u,f}$ nonequivalent f-IFDs; the minimum G-aberration f-IFD constructed from D_0 then can be identified.

In Step 1, we only consider the $1 \times e$ vector L rather than the complete $1 \times (2^u - 1)$ vector of length of words from the basic word when $e < 2^u - 1$. This makes the algorithm more efficient. In Step 2, we consider just one representative $\tilde{z}$ from each group, since the f-IFDs based on the same group must be equivalent. Next, we illustrate Algorithm 1 with the case of $u = 6$ and $f = 5$.

Example 5 (Example 4 continued)**.** To obtain the minimum G-aberration 6-IFD based on design 10.4, we need to consider 1176357 nonequivalent IFDs from different groups. We calculate Z-vectors of all these nonequivalent IFDs and obtain the unique absolute Z-vectors. Matching them to the lengths and J-characteristics of design 10.4's words, and obtain the confounding frequency vectors of all these nonequivalent IFDs. In this way, we obtain the minimum G-aberration 6-IFD based on design 10.4, defined by the foldover matrix

$$\Gamma = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 \end{bmatrix}.$$

It is easily checked the column $(1, 1, 1, 1, 1, 1)^T$ appears four times with indexes $1, 2, 4$ and 7 in Γ. This is consistent with the fact that the first 4 factors that can not be generated by the 6 basic words of design 10.4 are x_1, x_2, x_4 and x_7. The 6-IFD has CFV=$[(0, 0, 0, 0, 18, 0)_4]$, GR=4.67 and $B_4 = 2$.

By Algorithm 1, for any given initial design, one can obtain all nonequivalent f-IFDs and get the best one, provided u and f are not too large. When u and/or f is large,

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however, it can be computationally infeasible due to both time and space complexity, as the enumeration of equivalent groups increases sharply as u and f increase. For this reason, we next develop a shortcut to find the lowest G-aberration f-IFD from any initial design D_0.

For an f-IFD, its confounding frequency vector corresponding to $\tilde{z}$ is essentially determined by its B matrix. For matrix B, we use the coordinate exchange algorithm (Meyer and Nachtsheim, 1995) to search for the lowest G-aberration f-IFD based on D_0. Notably, the resulting design is the locally optimal solution, which may or may not be the globally optimal solution in terms of the G-aberration criterion. For this reason, we then use variable neighborhood search to optimize B for potential improvement. Variable neighborhood search is a popular optimization method that systematically explores multiple neighborhoods, where a neighborhood is defined to be some variants of a given solution (Mladenović and Hansen, 1997; Hansen and Mladenović, 2001; Hansen et al., 2008). Variable neighborhood search uses more than one neighborhood to prevent the search process from getting stuck in a locally optimal solution, as a locally optimal solution with respect to one neighborhood is not necessarily a locally optimal solution with respect to another neighborhood.

We now propose a second algorithm to search for the lowest G-aberration f-IFD for this situation, as given in Algorithm 2. Unlike the exhaustive search in Algorithm 1, Algorithm 2 finds the lowest G-aberration f-IFD by iteratively optimizing a random f-IFD and thus provides a shortcut to search for the lowest G-aberration f-IFD.

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Algorithm 2 (A short-cut to find a low G-aberration f-IFD)**.**

Input: A design with n runs and k factors called D_0, and an integer $f \geq 2$.

Output: The lowest G-aberration f-IFD constructed from D_0.

Step 1. For an initial n-run and k-factor design D_0, let $L = (L_1, \ldots, L_e)$ and $J = (J_1, \ldots, J_e)$ be the lengths and J-characteristics of words W arranged in Yates order, respectively.

Step 2. Randomly generate an $u \times (f-1)$ matrix on $\{-1, 1\}$, and set the corresponding f-IFD as the start. Obtain a locally optimal f-IFD through a coordinate exchange algorithm based on this start. Randomly choose M designs in the neighborhoods N_2 and N_3 of the locally optimal f-IFD, where N_i consists of f-IFDs whose B matrices differ from that of the local optimal design in exactly i positions for $i = 2, 3$.

Step 3. For each of the M designs, conduct the coordinate exchange algorithm and get the least G-aberration f-IFD. Choose the best one from all resulting f-IFDs to obtain the best f-IFD based on D_0.

Remark 1. Algorithms 1 and 2 can also be used to search for the lowest G_2-aberration f-IFD by changing the optimality objective from the confounding frequency vector to the generalized wordlength pattern.

Example 6. We seek the lowest G-aberration 6-IFD based on design 10.48. As discussed in Example 4, there are $4.7454 * 10^{10}$ nonequivalent 6-IFDs based on design 10.48, making Algorithm 1 computationally infeasible (due to both time and space complexity). We use the short-cut Algorithm 2. First, we randomly generate a 9×5 matrix with entries from $\{-1, 1\}$. It is then used as the B matrix of the starting 6-IFD after adding a 9×1 vector with all elements unity. Second, optimize the matrix B by the coordinate exchange to get a locally optimal 6-IFD based on this start. Then we apply the coordinate exchange to the randomly selected M =100 6-IFDs in the neighborhoods N_2 and N_3 of this local optimal 6-IFD. In this way, we obtain the lowest G-aberration 6-IFD based on design 10.48, defined by the foldover matrix

$$\Gamma = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 \end{bmatrix}.$$

It is easily checked that all elements in the fifth column of Γ are 1. This is consistent with the fact that factor x_5 can not be generated by the 9 basic words of design 10.48 (see Example 4 for the words of design 10.48). Besides, all elements in the sixth column of Γ are 1, indicating that like the fifth factor, this factor is not reversed in each of all 6 foldovers. The resulting design has CFV=$[(1, 0, 0, 0, 9, 32)_4]$, GR= 4 and $B_4 = 2.89$.

According to Examples 5 and 6, the 6-IFD for 10 factors in 96 runs from design 10.4 has less G- and G_2-aberration than that from design 10.48, while design 10.48 has less G- and G_2-aberration than design 10.4. For even f, the minimum G-aberration f-IFD often comes from a D_0 that is not the minimum aberration regular design.

Table 1: The Minimum G-aberration 6-IFDs based on 16×10 designs.

Initial design					Optimal	Minimum G-aberration 5-IFD	
Design	GR	CFV:$(f_{16}, f_8)_i$	u	F_0	foldover matrix	GR	CFV:$(f_{96}, f_{80}, f_{64}, f_{48}, f_{32}, f_{16})_4$
10.44	3.5	$[(4,24)_3,(3,48)_4]$	9	$\{7\}$	Γ_1	4.67	$[(0,0,0,0,3,48)_4]$
10.69	3.5	$[(4,21)_3,(3,51)_4]$	9	$\{7\}$	Γ_2	4.67	$[(0,0,0,0,3,51)_4]$
10.68	3.5	$[(4,20)_3,(3,52)_4]$	9	$\{7\}$	Γ_3	4.67	$[(0,0,0,0,3,52)_4]$

The foldover matrix for the ith best 6-IFD is Γ_i, where Γ_i is provided in the Supplementary Material; The initial designs 10.44, 10.69 and 10.68 are provided in the Supplementary Material.

As mentioned in Section 2, Sun (1993) (as well as Schoen et al. (2010)) provided 78 nonisomorphic designs of size 16×10, denoted as $10.z$ for $z = 1, \ldots, 78$. We obtain the lowest G-aberration 6-IFD for each of these 78 D_0 using Algorithm 2, and show the results for the best three in Table 1. The minimum G-aberration 6-IFD comes from design 10.44. Compared to the same size designs from Vazquez and Xu (2019), Wang and Mee (2021) and Wang and Mee (2023), our 6-IFD from Algorithm 2 has less G-aberration. It has the same G_2-aberration as the design in Wang and Mee (2021), and both of them have less G_2-aberration than the design in Vazquez and Xu (2019) and Wang and Mee (2023). In addition, it has the same DF for two-factor interactions as the designs in Wang and Mee (2021) and Wang and Mee (2023), as shown in Table 2, where DF denotes degrees of freedom for two-factor interactions. The PFD structure of each design is listed in the last column of Table 2. The 6-IFD is constructed from design 10.44 (where design 10.44 is an 8-PFD) and thus is a 48-PFD. Our algorithm does not always return the minimum G-aberration design for a given size. Vazquez et al. (2022) found a nonregular design for 10 factors in 96 runs

Table 2: Comparison of the 96×10 designs from Algorithm 2, Vazquez and Xu (2019), Wang and Mee (2021) and Wang and Mee (2023).

Source	CFV:$(f_{96}, f_{80}, f_{64}, f_{48}, f_{32}, f_{16})_4$	B_4	GR	PFD structure
Vazquez and Xu (2019)	$[(0,0,0,0,30,0)_4]$	3.33	4.67	48-PFD
Wang and Mee (2021)	$[(0,0,0,0,15,0)_4]$	1.67	4.67	6-PFD
Wang and Mee (2023)	$[(0,0,0,0,18,0)_4]$	2.00	4.67	6-PFD
6-IFD from Algorithm 2	$[(0,0,0,0,3,48)_4]$	1.67	4.67	48-PFD

All designs have DF=45 for two-factor interactions; Only the design from Vazquez and Xu (2019) has repeat runs, where it has 2 duplicate runs; The initial design of the 6-IFD, i.e. design 10.44 provided in the Supplementary Material, is an 8-PFD.

with CFV=$[(0,0,0,0,0,24)_4]$ and $B_4 = 0.67$ by concatenating two 48-run strength-three designs via an effective column change/variable neighborhood search algorithm. It is worth noting that our 6-IFD is a 48-PFD and thus much easier to understand and analyze. For example, the estimated models have a block diagonal information matrix where estimates of parameters belonging to different diagonal submatrices are uncorrelated. As such, the covariance matrix of the least-square estimates is simplified and the complexity of linear dependencies among factor effects is reduced. Therefore, aliasing relations are much easier to understood, which carries implications for both design choice and data analysis (Edwards and Mee, 2023). We believe that this is an important advantage over the alternative designs.

Note that the proposed 6-IFD is a 48-PFD based on a single flat of size 2. For the initial 2^{10-9} regular design, there is a total of 512 disjoint single flats in its family, with each determined by the sign assignment of 9 defining words. To obtain a 48-PFD, we

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include the first flat with +1 for all defining words, and consider the assignment of the other 47 flats from the remaining 511 flats; there are $511!/[47!564!] = 8.6 \times 10^{66}$ such cases to consider. An exhaustive search here is infeasible. A simulation study, provided in the Appendix, shows that the 48-PFD we constructed as a 6-IFD is extremely rare among numerous cases.

Similarly, we obtain the minimum G-aberration 10-IFD from design 10.z can be obtained for $z = 1, \ldots, 78$.Compared to the equally-sized designs from Vazquez and Xu (2019) and Wang and Mee (2023), the resulting 10-IFD has less G- and G_2-aberration with the same DF, as shown in Table 3. The 10-IFD is constructed from design 10.44 (where design 10.44 is an 8-PFD) and thus is an 80-PFD.

Table 3: Comparison of the 160×10 designs from Algorithm 2, Vazquez and Xu (2019) and Wang and Mee (2023).

Source	CFV:$(f_{160}, \ldots, f_{48}, f_{32}, f_{16})_4$	B_4	GR	PFD structure
Vazquez and Xu (2019)	$[(0,0,0,0,0,0,0,0,50,0)_4]$	2.00	4.8	80-PFD
Wang and Mee (2023)	$[(0,0,0,0,0,0,0,0,18,0)_4]$	0.72	4.8	10-PFD
10-IFD from Algorithm 2	$[(0,0,0,0,0,0,0,0,3,48)_4]$	0.60	4.8	80-PFD

All designs have DF=45 for two-factor interactions; Only the design from Vazquez and Xu (2019) has repeat runs, where it has 2 quadruplicate runs; The initial design of the 10-IFD, i.e. design 10.44 provided in the Supplementary Material, is an 8-PFD.

Example 7. As discussed in Wang and Mee (2023), their perturbation improvement algorithm does not always return the minimum G-aberration design for a given single flat. For instance, there exists an 8-PFD for 15 factors in 128 runs with generalized resolution 5.5, based on the minimum aberration 2^{15-11} design as single flat (Mee, 2009,

Table 4: Comparison of the 128×15 designs from Algorithm 2 and Wang and Mee (2023).

Source	CFV:$(f_{128}, f_{96}, f_{64}, f_{32})_4$	B_4	GR	PFD structure
Wang and Mee (2023)	$[(0, 0, 52, 0)_4]$	13.00	4.50	8-PFD
4-IFD from Algorithm 2	$[(0, 0, 0, 333)_4]$	20.81	4.75	32-PFD$^{\downarrow(2,32)}$

Both designs have no repeat runs; The initial design of the 4-IFD (provided in the Supplementary Material) is a 32-PFD; $^{\downarrow(\lambda,\mu)}$: The corresponding IFD can be reduced into a λ-IFD with the initial design being a μ-PFD.

Page 286). The best design they generate has a generalized resolution of 4.5. Using Algorithm 2, a 128×15 design with a generalized resolution of 4.75 can be obtained as a 4-IFD, where the initial 32×15 design is provided in the Supplementary Material. As summarized in Table 4, compared with the design from Wang and Mee (2023), the 4-IFD from Algorithm 2 has less G- and G_2-aberration as well as a larger generalized resolution. We can check that the 4-IFD can be reduced to a 2-IFD with the initial design being a 64-run 32-PFD. Following Theorem 3, the 4-IFD is a 32-PFD.

Technically, designs of size 100 can be constructed from a low-resolution single flat of size 4 as 25-PFDs, as described in Wang and Mee (2021, 2023). It is worth noting that constructing 5-IFDs from one of the 20-run orthogonal arrays is more successful. Let us consider the following illustrative example.

Example 8. A design with 100 runs and k factors can be constructed from the minimum aberration $2^{k-(k-2)}$ design as a 25-PFD. Note that the number of flats is large, and thus the construction methods in Wang and Mee (2021) are not feasible. Here we seek the minimum G-aberration 20-PFD via the perturbation improvement algorithm in Wang and Mee (2023). The $100 \times k$ design can also be constructed from the minimum G-aberration nonregular $20 \times k$ design as a 5-IFD via Algorithm 2. The initial nonregular designs are available in Eendebak and Schoen (2017). Table 5 summarizes the resulting $100 \times k$ designs from both methods for $k = 7, \ldots, 15$. Compared with the 25-PFD, the 5-IFD has less G-aberration and G_2-aberration, as well as a larger generalized resolution. In summary, the 5-IFDs from the 20-run nonregular design are superior to the 25-PFDs from the low-resolution 4-run single flat in terms of the G-aberration and G_2-aberration criteria. For k larger than 9, one might prefer the 25-PFD with a small $B_2 > 0$ to estimate more interactions.

These examples illustrate the merits of IFDs. That is, constructing good IFDs based on a nonregular initial design is often more successful than doing so with a more granular single flat. The IFD structure provides an efficient way to find good designs. Moreover, the resulting IFDs can be characterized as PFDs and thus are much easier to understand and analyze than many other nonregular designs (Edwards and Mee, 2023). One distinction of IFDs is that they may have partial replication. While single flats from the same family are either disjoint or identical, this is not the case for distinct foldovers of a given initial design. For instance, consider the two 100×7 designs in Example 8, as shown in Table 5. The one from Wang and Mee (2023) is a 25-PFD with 92 distinct rows. It has 23 distinct flats, two of which are repeated twice. The 5-IFD generated via Algorithm 2 has 88 distinct rows, 12 of which are repeated twice. Here partial replication is attractive because it provides the degrees of freedom for estimating the error variance.

Table 5: Comparison of the $100 \times k$ designs from Algorithm 2 (5-IFDs) and Wang and Mee (2023) (25-PFDs).

	5-IFD from the minimum G-aberration $20 \times k$ designs					25-PFD from the minimum aberration $2^{k-(k-2)}$ single flat				
k	CFV:$(f_{100}, \ldots, f_{12}, f_4)_i$	(B_2, B_3)	GR	DF	κ	CFV:$(f_{100}, \ldots, f_{20}, f_{12}, f_4)_i$	(B_2, B_3)	GR	DF	κ
7	$[(0, \ldots, 0, 0)_2, (0, \ldots, 0, 35)_3]$	(0,0.056)	3.96	21	12	$[(0, \ldots, 0, 5)_2, (0, \ldots, 0, 0, 12)_3]$	(0.008,0.0192)	2.96	21	8
8	$[(0, \ldots, 0, 0)_2, (0, \ldots, 0, 56)_3]$	(0,0.0896)	3.96	28	12	$[(0, \ldots, 0, 7)_2, (0, \ldots, 0, 0, 18)_3]$	(0.0112,0.0288)	2.96	28	4
9	$[(0, \ldots, 0, 0)_2, (0, \ldots, 0, 84)_3]$	(0, 0.1344)	3.96	36	4	$[(0, \ldots, 0, 9)_2, (0, \ldots, 0, 0, 27)_3]$	(0.0144,0.0432)	2.96	36	–
10	$[(0, \ldots, 0, 0)_2, (0, \ldots, 0, 120)_3]$	(0, 0.1920)	3.96	42	–	$[(0, \ldots, 0, 12)_2, (0, \ldots, 0, 0, 36)_3]$	(0.0192,0.0576)	2.96	45	–
11	$[(0, \ldots, 0, 0)_2, (0, \ldots, 5, 160)_3]$	(0, 0.3280)	3.88	50	–	$[(0, \ldots, 0, 15)_2, (0, \ldots, 0, 7, 41)_3]$	(0.0240,0.1664)	2.96	55	–
12	$[(0, \ldots, 0, 0)_2, (0, \ldots, 8, 212)_3]$	(0, 0.4544)	3.88	56	–	$[(0, \ldots, 0, 18)_2, (0, \ldots, 0, 10, 54)_3]$	(0.0288,0.2304)	2.96	66	–
13	$[(0, \ldots, 0, 0)_2, (0, \ldots, 14, 272)_3]$	(0,0.6368)	3.88	57	–	$[(0, \ldots, 0, 22)_2, (0, \ldots, 0, 12, 64)_3]$	(0.0352,0.3328)	2.96	74	–
14	$[(0, \ldots, 0, 0)_2, (0, \ldots, 20, 344)_3]$	(0,0.8384)	3.88	57	–	$[(0, \ldots, 0, 26)_2, (0, \ldots, 5, 41, 51)_3]$	(0.0416,0.8768)	2.96	83	–
15	$[(0, \ldots, 0, 0)_2, (0, \ldots, 26, 429)_3]$	(0,1.0608)	3.88	57	–	$[(0, \ldots, 0, 30)_2, (0, \ldots, 6, 51, 68)_3]$	(0.0480,1.0832)	2.96	81	–

All 5-IFDs are 100-PFDs; κ: The corresponding design has κ duplicate runs; –: The corresponding design has no repeat runs.

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5. Summary and discussion

This article introduces a new class of nonregular designs called IFDs, that is composed of several foldovers of an initial design. We study the general theory for IFDs, and present a method to obtain all nonequivalent f-IFDs for any given initial design. Two algorithms were given to search for the optimal f-IFD in terms of G-aberration (or G_2-aberration) criterion. It is worth noting that IFDs have a parallel flats structure, and thus are much easier to understand and analyze than many other nonregular designs. Most importantly, as illustrated in Tables 2–5, constructing good IFDs based on a nonregular initial design is often more successful than doing so with a more granular single flat. The IFD structure provides an efficient way to find good designs.

The IFDs include several existing designs as special cases. When f is 2, and the initial design D_0 is taken to be a regular design, the resulting 2-IFDs degenerate to the combined designs in Li and Lin (2003); When f is 2, and the initial design D_0 is taken to be a nonregular design, the resulting 2-IFDs degenerate to the combined designs in Li et al. (2003). More construction results are provided in the Appendix.

Supplementary Material

The online Supplementary Material includes S1: the proofs of Theorems 1–3 and Corollaries 1 and 2; S2: the optimal foldover matrices for the three 6-IFDs in Table 1; S3: the initial designs of the IFDs in Tables 1–4; S4: the initial designs of the IFDs in Tables C.1 and C.2; and S5: The indicator function of design 10.48.

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Appendix

Appendix A: An illustrative example of the basic words

Let H_{12} be the 12×11 Plackett-Burman design, which is provided in the Supplementary Material. It has in total of 1123 words, i.e. one complete word, 990 partial words of aliasing index 1/3, and 132 partial words of aliasing index 2/3. It is a 12-PFD, where the single flat can be regared as the 2^{11-11} design with $2^{11} - 1 = 2047$ complete words generated by $X = \{x_1, x_2, \ldots, x_{11}\}$. Among the 2047 complete words of the single flat, 990 words become partial words of aliasing index 1/3, 132 words become partial words of aliasing index 2/3, one word remains a complete word, and the remaining 924 words are removed in design H_{12}. The 1123 words of design H_{12} can be generated by the 11 words in X. Thus, we have $n = 12$, $k = 11$, $g = 12$, $e = 1123$ and $u = 11$ for design H_{12}. Here $g = n$, $u = k$ and $e < 2^u - 1$.

Take the first 10 columns of H_{12} and denote the resulting 12×10 design as H_{12}^{10}. We can check that H_{12}^{10} is a 12-PFD. It has 495 partial words of aliasing index 1/3 and 66 partial words of aliasing index 2/3. The 561 words can be generated by the 10 words in $X = \{x_1, x_2, \ldots, x_{10}\}$. Thus, we have $n = 12, k = 10, g = 12$, $e = 561$ and $u = 10$ for design H_{12}^{10}. Here $g = n$, $u = k$ and $e < 2^u - 1$.

Table A.1: The basic words of designs H_{12}^k for $k = 3, \ldots 11$.

k	g	e	u	CFV:$(f_{12}, f_8, f_4)_i$
3	3	1	1	$[(0,0,1)_3]$
4	12	5	4	$[(0,0,4)_3], (0,0,1)_4]$
5	12	15	5	$[(0,0,10)_3, (0,0,5)_4, (0,0,0)_5]$
6	12	36	6	$[(0,0,20)_3, (0,0,15)_4, (0,1,0)_5, (0,0,0)_6]$
7	12	75	7	$[(0,0,35)_3, (0,0,35)_4, (0,3,0)_5, (0,1,0)_6, (0,0,1)_7]$
8	12	147	8	$[(0,0,56)_3, (0,0,70)_4, (0,8,0)_5, (0,4,0)_6, , (0,0,8)_7, (0,0,1)_8]$
9	12	285	9	$[(0,0,84)_3, (0,0,126)_4, (0,18,0)_5, (0,12,0)_6, (0,0,36)_7, (0,0,9)_8, (0,0,0)_9]$
10	12	561	10	$[(0,0,120)_3, (0,0,210)_4, (0,36,0)_5, (0,30,0)_6, (0,0,120)_7, (0,0,45)_8, (0,0,0)_9, (0,0,0)_{10}]$
11	12	1123	11	$[(0,0,165)_3, (0,0,330)_4, (0,66,0)_5, (0,66,0)_6, (0,0,330)_7, (0,0,165)_8, (0,0,0)_9, (0,0,0)_{10}, (0,0,1)_{11}]$

The $12 \times k$ design H_{12}^k is a g-PFD with e words. It has u basic words. Here f_{i8}, f_{i4} correspond to partial words of aliasing index 2/3 and 1/3 respectively, while f_{i12} corresponds to complete words.

Let H_{12}^k be the $12 \times k$ design consisting of the first k columns of H_{12}. Table A.1 lists the k (number of factors), g (number of flats), e (number of words), u (number of basic words) and CFV of design H_{12}^k for $k = 3, \ldots, 12$. As shown in Table A.1, for $k = 4, \ldots, 11$, design H_{12}^k is a 12-PFD, and thus $u = k$. Design H_{12}^3 has one partial word of aliasing index 1/3. This design is a 3-PFD, where the single flat is a 2^{3-1} design with one complete word $x_1x_2x_3$. This word becomes a partial word of aliasing index 1/3 of design H_{12}^3 as a 3-PFD. Thus, we have $n = 12$, $k = 3$, $g = 3$, $u = 1$, $e = 1$ for design H_{12}^3 with $u = k - \log_2(n/g)$. Here $e = 2^u - 1$ holds even though design H_{12}^3 is nonregular.

Appendix B: A simulation example used to supplement Table 2

Here we show that the 48-PFD we constructed as a 6-IFD is extremely rare among all possible 48-PFDs from the 2^{10-9} single flat. To see this, we evaluate 100000 48-PFDs generated by the perturbation improvement algorithm in Wang and Mee (2023). The generalized resolutions of these designs are 2.91, 2.96, 4.33, 4.50, and 4.67 with frequencies of 728, 98971, 1, 148, and 152, respectively. There are in total of 301 strength-three designs and their B_4 values are distributed as in Figure B.1. The minimum G-aberration design has GR=4.67, $B_4 = 4.06$ and CFV=$[(0, 0, 0, 0, 0, 0, 0, 0, 9, 110)_4]$, while the minimum G_2-aberration design has GR=4.67, $B_4 = 3.92$ and CFV=$[(0, 0, 0, 0, 0, 0, 0, 0, 11, 97)_4]$. None of these 100000 48-PFDs achieve a B_4 of 1.67, not even close. That is, the proposed 6-IFD which can be characterized as a 48-PFD, is superior to the 100000 48-PFDs under both G- and G_2-aberration criteria. Note that any 6-IFD can form a 48-PFD. Thus the set of all 6-IFDs will be a subset of all 48-PFDs. It is clear that the search for 6 foldovers of size 16 is easier than the search for 48 flats of size 2. The simulation study indicates that the 48-PFDs that are not included in the subset defined by 6-IFDs do not contain any designs better than the best 6-IFD.

Appendix C: Some IFDs from Algorithm 2

Some selected isomorphic foldovers designs constructed from the 12×11 and 16×15 designs are listed in Tables C.1 and C.2 respectively. The initial designs i.e. the unique 12×11 strength-two design (Plackett-Burman design) and five nonisomorphic 16×15 strength-two designs are available in Sun (1993), Schoen et al. (2010), Eendebak and Schoen (2017) and the library of orthogonal arrays maintained by Dr. N.J.A. Sloane

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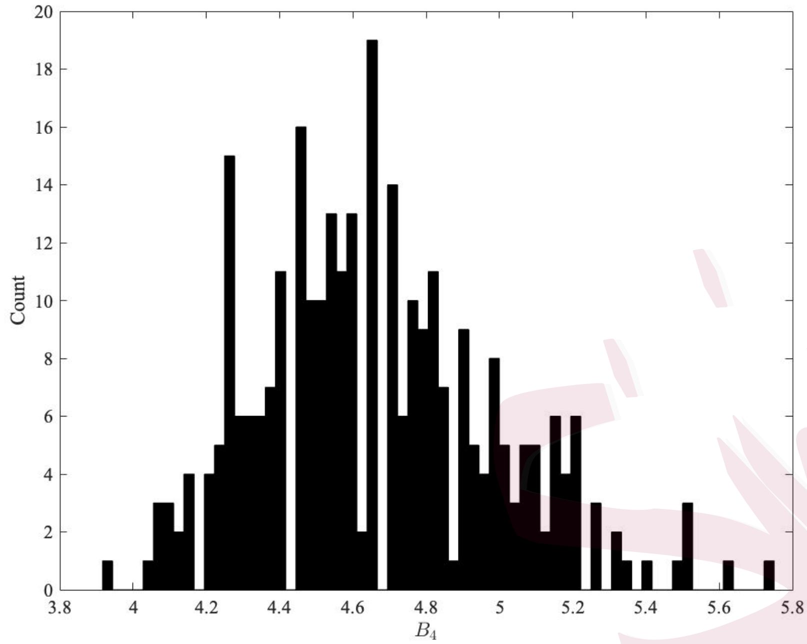

Figure B.1: The distribution of B_4 of the 301 strength-three 48-PFDs.

(http://neilsloane.com/oadir/index.html). We provide these designs in the Supplementary Material. As shown in Tables C.1 and C.2, all the IFDs have a parallel flats structure. For $f = 4, 6, 8, 10$, the f-IFD based on the 12-run Plackett-Burman design can be reduced into a $(f/2)$-IFD, where the initial design is a 2-IFD based on the Plackett-Burman design, as shown in the last column of Table C.1.

Table C.1: Selected f-IFDs from the 12×11 strength-two design.

Runs	f	CFV=$(f_{48}, f_{40}, f_{32}, f_{24}, f_{16}, f_8)_4$	B_4	GR	DF	PFD structure
24	2	$[(0, 0, 0, 0, 0, 330)_4]$	36.67	4.67	11	12-PFD
48	4	$[(0, 0, 0, 0, 154, 0)_4]$	17.11	4.67	22	12-PFD$^{\downarrow(2,12)}$
72	6	$[(0, 0, 0, 70, 0, 260)_4]$	10.99	4.67	33	36-PFD$^{\downarrow(3,12)}$
96	8	$[(0, 0, 28, 0, 168, 0)_4]$	7.78	4.67	44	48-PFD$^{\downarrow(4,12)}$
120	10	$[(0, 8, 0, 102, 0, 220)_4]$	5.95	4.67	53	60-PFD$^{\downarrow(5,12)}$
144	12	$[(2, 0, 66, 0, 168, 0)_4]$	5.56	4.67	55	72-PFD$^{\downarrow(6,12)}$

The initial 12×11 strength-two design (provided in the Supplementary Material) is a 12-PFD; All IFDs have no repeat runs; $^{\downarrow(\lambda,\mu)}$: The corresponding IFD can be reduced into a λ-IFD with the initial design being a μ-PFD.

Table C.2: Selected f-IFDs from 16×15 strength-two designs.

Runs	f	D_0	CFV=$(f_{96}, f_{80}, f_{64}, f_{48}, f_{32}, f_{16})_4$	B_4	GR	DF	PFD structure
32	2	$H_{16.V}$	$[(0, 0, 0, 0, 21, 336)_4]$	105.00	4.00	15	8-PFD
64	4	$H_{16.III}$	$[(0, 0, 9, 0, 144, 0)_4]$	45.00	4.00	30	8-PFD$^{\downarrow(2,8)}$
96	6	$H_{16.II}$	$[(3, 0, 0, 48, 54, 144)_4]$	25.00	4.00	45	12-PFD$^{\downarrow(3,4)}$
128	8	$H_{16.I}$	$[(0, 0, 32, 0, 0, 0)_4]$	8.00	4.50	81	8-PFD
160	10	$H_{16.V}$	$[(3, 8, 0, 102, 18, 226)_4]$	15.24	4.40	75	40-PFD$^{\downarrow(5,8)}$

The initial 16×15 designs labeled $H_{16.I}, \ldots, H_{16.V}$ (provided in the Supplementary Material) are 1, 4, 8, 16, and 8-PFD respectively; All IFDs have no repeat runs; $^{\downarrow(\lambda,\mu)}$: The corresponding IFD can be reduced into a λ-IFD with the initial design being a μ-PFD.

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