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A Three-Quarter Fold-Over Strategy for Follow-Up Designs in Fractional Factorial Experiments

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Abstract: Follow-up design is a fundamental problem in statistical design of experiments, especially in fractional factorial designs, where aliasing among effects can obscure interpretation and reduce design efficiency. The fold-over technique is commonly used to address this issue by augmenting the initial design with additional runs obtained by switching the levels of one or more factors. In this paper, a new methodology for constructing follow-up designs based on a fold-over approach is proposed and investigated. The performance of the constructed design is evaluated using several statistical design-ranking criteria. The results show that the proposed design achieves higher D-efficiency (up to approximately 98%) and lower average prediction variance than the initial and semi-fold-over designs, indicating more efficient estimation and improved prediction performance..

Keywords: fold-over design, fractional factorial design, D-efficiency, average prediction variance (APV), estimation capacity (EC)

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1. Introduction

One of the main challenges in fractional factorial designs is the aliasing among effects, which can obscure interpretation and reduce the efficiency of the design. A common strategy for addressing this issue is the fold-over technique, which is widely used to construct follow-up experiments. This technique involves reversing the signs of one or more factors in the initial design and augmenting the original runs, thereby improving the resolution and estimation capability of the design. When a full fold-over is applied to a resolution III design by reversing the signs of all factor columns, a resolution IV design is obtained. In such designs, two-factor interactions are confounded with three-factor interactions, which are often assumed to be negligible. Alternatively, a fractional fold-over may be applied by reversing selected factors only, providing greater flexibility in isolating specific effects. For further details, see Montgomery (2017).

Several studies have investigated optimal fold-over strategies for fractional factorial design. Li and Lin (2003) investigated optimal fold-over plans for two-level fractional factorial designs under the minimum aberration (MA) criterion and analyzed their properties using indicator functions (Fries and Hunter, 1980). For nonregular designs, Li et al. (2003) extended this work by proposing optimal fold-over strategies under the generalized minimum aberration (GMA) criterion (Deng and Tang, 2002). These studies highlight the complexity of aliasing structures, particularly in nonregular designs.

The semi-fold-over technique was introduced by Barnett et al. (1997) as a strategy for augmenting the initial design with only half of the runs in the full fold-over design rather than with the complete run size. This approach enables the isolation of important main effects and two-factor interactions while reducing experimental resources (Mee and Peralta, 2000). However, Mee and Peralta (2000) also noted that full fold-over designs with resolution IV are often inefficient in terms of degrees of freedom, as they may provide fewer than $n/2$ additional degrees of freedom for estimating two-factor interactions. To address these limitations, Edwards (2014) proposed an alternative strategy, known as the double semi-fold-over, which is constructed by adding two semi-fold-over fractions to the initial design. This method allows more effects to be estimated than the standard fold-over technique. Furthermore, Liau (2021) presented illustrative examples of semi-fold-over and double semi-fold-over strategies for several experimental designs.

Although fold-over and semi-fold-over design strategies have been used extensively in follow-up experimentation, they still have important limitations. The classical fold-over technique requires augmenting the initial design with an additional design of equal size, resulting in a combined design with twice the number of runs. This increases experimental cost and resource consumption, making the approach inefficient in many practical situations. Although semi-fold-over and double semi-fold-over designs reduce the number of additional runs relative to the full fold-over, they often suffer from residual aliasing, particularly among two-factor interactions, and may exhibit inconsistent performance across design evaluation criteria.

Therefore, more flexible and efficient follow-up design strategies are needed to improve the estimability of interaction effects without substantially increasing the number of experimental runs. To address this gap, this study proposes a three-quarter fold-over design strategy that balances full fold-over and semi-fold-over approaches. The proposed method aims to improve the efficiency of follow-up designs while controlling the number of additional runs. Its effectiveness is evaluated using multiple criteria, including estimation capacity (EC), D-efficiency, and average prediction variance (APV), and is compared with the initial design and existing semi-fold-over techniques.

The remainder of this paper is organized as follows. Section 2 reviews the design evaluation criteria, namely estimation capacity (EC), D-efficiency, and average prediction variance (APV), and explains their relevance for assessing design performance. Section 3 presents the proposed methodology. Section 4 reports the results. Section 5 provides the discussion and concluding remarks.

2. Preliminaries

To evaluate the effectiveness of the proposed design, this study adopts a set of complementary criteria selected to align with the main objective of improving the estimability of interaction effects. Specifically, estimation capacity (EC), D-efficiency, and average prediction variance (APV) are used to assess design performance from different perspectives. Together, these criteria provide a comprehensive evaluation of the estimation capability, statistical efficiency, and prediction performance.

2.1 Estimation Capacity

Estimation capacity (EC) was first introduced by Cheng et al. (1999) and is defined as the total number of estimable models that contain all k main effects and g two-factor interactions. Mee et al. (2017) further described the estimation capacity as a vector (EC_1,…, EC_G), in which each component represents the ratio of estimable models to the total number of possible models with the same structure. Formally, the estimation capacity for g two-factor interactions is defined as:

$$EC_g = \frac{N_g^e}{N_g}, g = 1,2, \ldots . G$$

where N_g^e denotes the number of estimable models containing all k main effects and g two-factor interactions, and N_g denotes the total number of possible models with the same structure. The total number of possible two-factor interactions among k factors is $\binom{k}{2}$; therefore, the total number of candidate models with exactly g interactions is given by:

$$N_g = \binom{\binom{k}{2}}{g}$$

A design is considered effective if all components of the estimation capacity vector reach their maximum value of 1. This criterion is particularly appropriate for evaluating the proposed design because it directly reflects the design's ability to identify and estimate models that include main effects and two-factor interactions. In this sense, estimation capacity provides a meaningful measure of the estimability of the underlying models supported by the design.

2.2 D-efficiency

D-efficiency is derived from the D-optimality criterion introduced by Kiefer and Wolfowitz (1959), which focuses on maximizing the determinant of the information matrix $X'X$ to ensure precise estimation of model parameters (Montgomery, 2013). As a normalized version of this criterion, D-efficiency provides a scale-invariant measure that enables comparisons among designs of different sizes. It is commonly expressed as:

$$D = \left(\frac{det(X'X)}{n^p}\right)^{\frac{1}{p}}$$

where X is the design matrix, n is the number of experimental runs, and p is the number of model parameters. This formulation reflects the amount of information contained in the design relative to its size (Atkinson et al., 2007; Myers et al., 2016).

This criterion is particularly appropriate for evaluating the proposed design because it quantifies the design's ability to provide precise and stable parameter estimates. A higher D-efficiency indicates a more informative design and therefore reflects the overall quality and effectiveness of the design in parameter estimation.

2.3 Average Prediction Variance

Average prediction variance (APV) was first introduced by Box and Draper (1987). It represents the average variance of the predicted responses over the experimental region. A smaller APV value indicates better prediction performance. Simmons (2023) used APV to compare and evaluate different designs before conducting experiments and showed, both theoretically and through simulation studies, that designs with lower APV provide better prediction accuracy.

The APV is based on the variance of the predicted response. According to Montgomery (2013), the variance of the predicted response at a point x is given by:

$$Var(\hat{y}(x)) = \sigma^2 x'(X'X)^{-1}x$$

where X is the design matrix. APV is obtained by averaging this variance over the design region.

This criterion is appropriate for evaluating the proposed design because it reflects the design's ability to provide accurate and stable predictions across the experimental region. In this sense, APV serves as a useful measure of the design's prediction capability.

3. Methodology for Constructing a Three-Quarter Fold-Over Design

This study proposes a structured procedure for constructing a three-quarter fold-over follow-up design. The methodology is formally defined as follows.

Step 1. Let D denote the initial design matrix with n runs and k main effects. Select a factorial effect $\chi \in D$ whose levels will be reversed to introduce a structured modification to the original design.

Step 2. Construct the fold-over design, denoted by D_x, by reversing the signs of the selected factor x. The combined design is then obtained as: $S=D \cup D_x$, which reduces aliasing between main effects and interaction effects.

Step 3. To further refine the design, apply a subsetting procedure to S based on two selected effects (either a main effects and one two-factor interaction, or two two-factor interactions), resulting in four equal-sized subsets, S_i, i=1,2,3,4 such that $S = S_1 \cup S_2 \cup S_3 \cup S_4$. This partitioning facilitates the systematic selection and exclusion of subsets.

Step 4. Select any three subsets and combine them with the original design D to construct the final three-quarter fold-over design: $D^* = D \cup S_a \cup S_b \cup S_c$, where $\{a, b, c\} \subset \{1, 2, 3, 4\}$. This step balances design size and estimation capability by incorporating 75% of the fold-over design, thereby improving estimability without using the full fold-over.

This construction balances full fold-over and semi-fold-over designs while controlling the number of additional experimental runs. The resulting design is evaluated using estimation capacity (EC), D-efficiency, and average prediction variance (APV), as defined in the previous section.

For illustration, consider a 2^{5-1} fractional factorial design defined by the generator E = ABC, resulting in an initial design with 16 runs. A fold-over is performed on factor C. Subsetting is then applied based on the effects E and AB, which partitions the design into four equal-sized subsets. A three-quarter fold-over design is constructed by augmenting the initial 16-run design with three of these subsets, resulting in a total of 28 runs. The proposed construction procedure is illustrated in Figure 1.

	A	B	C	D	E
1	-1	-1	-1	-1	-1
2	1	-1	-1	-1	1
3	-1	1	-1	-1	1
4	1	1	-1	-1	-1
5	-1	-1	1	-1	1
6	1	-1	1	-1	-1
7	-1	1	1	-1	-1
8	1	1	1	-1	1
9	-1	-1	-1	1	-1
10	1	-1	-1	1	1
11	-1	1	-1	1	1
12	1	1	-1	1	-1
13	-1	-1	1	1	1
14	1	-1	1	1	-1
15	-1	1	1	1	-1
16	1	1	1	1	1

(a) Initial design

	A	B	C	D	E
1	-1	-1	1	-1	1
2	1	-1	1	-1	-1
3	-1	1	1	-1	-1
4	1	1	1	-1	1
5	-1	-1	-1	-1	-1
6	1	-1	-1	-1	1
7	-1	1	-1	-1	1
8	1	1	-1	-1	-1
9	-1	-1	1	1	1
10	1	-1	1	1	-1
11	-1	1	1	1	-1
12	1	1	1	1	1
13	-1	-1	-1	1	-1
14	1	-1	-1	1	1
15	-1	1	-1	1	1
16	1	1	-1	1	-1

(b) Fold-over on factor C

	A	B	C	D	E
1	-1	-1	-1	-1	-1
2	1	-1	-1	-1	1
3	-1	1	-1	-1	1
4	1	1	-1	-1	-1
5	-1	-1	1	-1	1
6	1	-1	1	-1	-1
7	-1	1	1	-1	-1
8	1	1	1	-1	1
9	-1	-1	-1	1	-1
10	1	-1	-1	1	1
11	-1	1	-1	1	1
12	1	1	-1	1	-1
13	-1	-1	1	1	1
14	1	-1	1	1	-1
15	-1	1	1	1	-1
16	1	1	1	1	1

(c) Partitioning based on E and AB

	A	B	C	D	E
1	-1	-1	-1	-1	-1
2	1	-1	-1	-1	1
3	-1	1	-1	-1	1
4	1	1	-1	-1	-1
5	-1	-1	1	-1	1
6	1	-1	1	-1	-1
7	-1	1	1	-1	-1
8	1	1	1	-1	1
9	-1	-1	-1	1	-1
10	1	-1	-1	1	1
11	-1	1	-1	1	1
12	1	1	-1	1	-1
13	-1	-1	1	1	1
14	1	-1	1	1	-1
15	-1	1	1	1	-1
16	1	1	1	1	1

(d) Combined design

Figure 1. Procedure for constructing the three-quarter fold-over design.

3.1 Alias Structure Considerations for Subsetting

To ensure valid subsetting, it is important to account for the design alias structure. In fractional factorial designs, the alias structure defines relationships among effects. For example, in the 2^(4-1) design with generator D=ABC, the alias structure implies relationships such as AB=CD, AD=BC, and BD=AC. Therefore, when selecting two-factor interactions for subsetting, effects should be chosen from different alias groups. Selecting equivalent interactions produce meaningful partitioning, whereas selecting interactions from different groups ensures distinct subsets. Similar aliasing patterns were observed across all considered designs.

This consideration directly affects the quality of the resulting subsets. Selecting interactions from different alias groups enhances the structural diversity of the design and improves its statistical properties, whereas selecting interactions from the same group leads to redundant partitions with limited benefit. Therefore, appropriate selection of subsetting effects is essential for achieving efficient and informative follow-up designs.

4. Results

Factorial designs with different resolutions were considered to evaluate the proposed three-quarter fold-over design. A single-factor fold-over strategy was applied by reversing factor C. The selection of factor C is arbitrary, and the same procedure can be applied to any main effect. Different subsetting schemes were also examined, including combinations of main effects with one two-factor interactions and schemes based solely on two two-factor interactions. The performance of the initial, semi-fold-over, and three-quarter fold-over designs was assessed in terms of D-efficiency, average prediction variance (APV), and estimation capacity (EC), as summarized in Table 1.

Table 1. Evaluation of the proposed three-quarter fold-over design compared with initial and semi-fold-over designs

Design	Generator	Fold-over strategy	Subsetting scheme	Number of runs	D-efficiency	APV	EC_3
$\overline{2^{4-1}_{initial}}$	D=ABC	--	--	8	100	0.291667	0.4
2^{4-1}_{semi}	D=ABC	C	D, AB	12	97.67187	0.20833	0.4
			AD, BC		95.39794	0.20833	0.4
$2^{4-1}_{three-quarter}$	D=ABC	C	D, AB	14	98.21554	0.173611	0.4
			AD, BC		96.86961	0.175595	0.4
$2^{5-2}_{initial}$	D=ABC, E=ABD	--	--	8	100	0.291667	0.4
$\overline{2^{5-2}_{semi}}$	D=ABC, E=ABD	C	A, BC	12	97.67187	0.20833	0.4
			AD, BD		95.39794	0.20833	0.4
$2^{5-2}_{three-quarter}$	D=ABC, E=ABD	C	A, BC	14	98.21554	0.173611	0.4
			AD, BC		96.86961	0.175595	0.4
$2^{5-1}_{initial}$	E=ABC	--	--	16	100	0.166667	0.8
2^{5-1}_{semi}	E=ABC	C	E, AB	24	98.05609	0.118056	0.8
			AB, BE		96.14997	0.118056	0.8
$2^{5-1}_{three-quarter}$	E=ABC	C	E, AB	28	98.51072	0.09871	0.8
			AB, BE		97.38445	0.099702	0.8
$\overline{2^{5-1}_{initial}}$	E=ABCD	--	--	16	100	0.166667	1
2^{5-1}_{semi}	E=ABCD	C	A, CD	24	98.05609	0.118056	1
			AE, CE		98.05609	0.114583	1
$2^{5-1}_{three-quarter}$	E=ABCD	C	A, CD	28	98.97433	0.097222	1
			AE, CE		98.84984	0.097024	1

Note: Table 1 reports estimation capacity up to three two-factor interactions. The values remain identical for cases involving up to seven interactions.

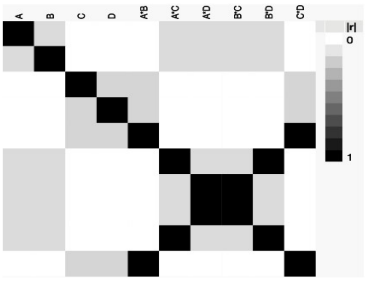
The results indicate that the proposed three-quarter fold-over design consistently improves D-efficiency compared to the semi-fold-over design across all considered cases. In terms of prediction performance, the proposed design yields lower APV values compared to both the initial and semi-fold-over designs. However, no improvement is observed in estimation capacity, as the EC values remain unchanged across all designs.

To further evaluate the robustness of the proposed design, a sensitivity analysis was conducted by considering different fold-over strategies while retaining the same subsetting schemes used in Table 1. The results are summarized in Table 2.

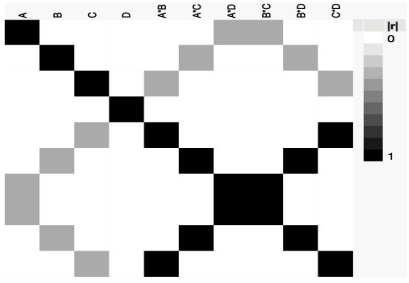
Table 2. Sensitivity analysis under different fold-over strategies

Design	Generator	Fold-over strategy	Subsetting scheme	Number of runs	D-efficiency	APV	EC_3
$\overline{2^{4-1}_{initial}}$	D=ABC	--	--	8	100	0.291667	0.4
2^{4-1}_{semi}	D=ABC	A, B, C, D	D, AB	12	97.67187	0.20833	0.4
			AD, BC		95.39794	0.20833	0.4
$2^{4-1}_{three-quarter}$	D=ABC	A, B, C, D	D, AB	14	98.21554	0.173611	0.4
			AD, BC		96.86961	0.175595	0.4
$2^{5-2}_{initial}$	D=ABC, E=ABD	--	---	8	100	0.291667	0.4
2^{5-2}_{semi}	D=ABC, E=ABD	A, B, C, D, E	A, BC	12	97.67187	0.20833	0.4
			AD, BD		95.39794	0.20833	0.4
$2^{5-2}_{three-quarter}$	D=ABC, E=ABD	A, B, C, D, E	A, BC	14	98.21554	0.173611	0.4
			AD, BC		96.86961	0.175595	0.4
$2^{5-1}_{initial}$	E=ABC	--	--	16	100	0.166667	0.8
2^{5-1}_{semi}	E=ABC	A, B, C, D, E	E, AB	24	98.05609	0.118056	0.8
			AB, BE		98.05609	0.118056	0.8
$2^{5-1}_{three-quarter}$	E=ABC	A, B, C, D, E	E, AB	28	98.51072	0.09871	0.8
			AB, BE		98.51072	0.099702	0.8
$2^{5-1}_{initial}$	E=ABCD	--	--	16	100	0.166667	1
2^{5-1}_{semi}	E=ABCD	A, B, C, D, E	A, CD	24	98.05609	0.118056	1
			AE, CE		98.05609	0.114583	1
$2^{5-1}_{three-quarter}$	E=ABCD	A, B, C, D, E	A, CD	28	98.97433	0.097222	1
			AE, CE		98.84984	0.097024	1

The results indicate that there is no noticeable difference between the full fold-over and single-factor fold-over strategies in terms of D-efficiency and APV. Both approaches yield similar values across the considered designs. However, the choice of subsetting effects has a clear impact on performance. Subsetting schemes that include both main effects and two-factor interactions result in higher D-efficiency, whereas schemes based solely on two-factor interactions lead to lower values. In addition, the aliasing among effects, particularly between main effects and two-factor interactions, was examined, as illustrated in Figure 2.



(a) Correlation map of the three-quarter fold-over



(b) Correlation map of the semi-fold-over

Alias Matrix

Effect	A*B	A*C	A*D	B*C	B*D	C*D
Intercept	-0.2	0	0	0	0	-0.2
A	0	-0.17	-0.17	-0.17	-0.17	0
B	0	-0.17	-0.17	-0.17	-0.17	0
C	-0.2	0	0	0	0	-0.2
D	-0.2	0	0	0	0	-0.2

(c) Aliasing matrix of the three-quarter fold-over

Alias Matrix

Effect	A*B	A*C	A*D	B*C	B*D	C*D
Intercept	0	0	0	0	0	0
A	0	0	-0.33	-0.33	0	0
B	0	-0.33	0	0	-0.33	0
C	-0.33	0	0	0	0	-0.33
D	0	0	0	0	0	0

(d) Aliasing matrix of the semi-fold-over

Figure 2. Correlation maps and aliasing matrices for three-quarter and semi-fold-over designs for 2^{4-1} design.

Figure 2 presents a representative example of the aliasing and correlation structure for the considered designs. Similar patterns were consistently observed across all designs; therefore, only one representative case is shown for clarity. The results indicate that the proposed three-quarter fold-over design reduces correlations among effects compared with the semi-fold-over design, resulting in a more stable design structure.

5. Discussion and Concluding

This study examines the performance of the proposed three-quarter fold-over design in fractional factorial experiments. The results, as reported in Table 1, show that the proposed design achieves higher D-efficiency and lower APV than the initial and semi-fold-over designs. However, no improvement is observed in estimation capacity. In addition, multicollinearity between main effects and two-factor interactions is observed, as illustrated in Figure 2. The results also show no noticeable effect of the fold-over strategy (single-factor versus full fold-over) on the evaluated criteria.

These findings can be understood through the properties of the information matrix $X'X$, where D-efficiency is related to its determinant and APV is linked to its inverse. In the considered cases, designs with larger run sizes show improved D-efficiency and lower APV, indicating more stable estimation and better prediction performance. This observation is consistent with the theory that increasing the run size improves the quality of the information matrix (Montgomery, 2017; Atkinson, 2025).

In contrast, no improvement is observed in estimation capacity across the considered designs. This indicate that estimation capacity depends on the alias structure of the design rather than on the number of runs. Therefore, the proposed design does not improve this criterion, as no additional independent information is introduced and the number of estimable models remains unchanged. This finding is consistent with the fundamental principle in fractional factorial designs that estimability is driven by the defining relation and alias structure rather than simply by increasing the number of experimental runs (Montgomery, 2017).

Moreover, the presence of multicollinearity in the proposed design can be attributed to the structure of the fold-over construction, particularly when partial fold-over strategies, such as semi- and three-quarter fold-over are used. As shown in Figure 2, the alias matrix highlights the correlation between main effects and two-factor interactions, indicating the presence of multicollinearity. When such correlations exist, the estimated coefficients become less stable. In practical terms, small changes in the data may lead to noticeable changes in the coefficient estimates, making it more difficult to interpret the individual effects of the factors. This is consistent with previous findings in the literature. For example, Montgomery (2017) explains that multicollinearity in fractional factorial designs arises from the aliasing structure, which can increase the variance of the estimates and reduce their interpretability. Similarly, regression analysis literature (e.g., Kutner et al., 2005) shows that multicollinearity inflates the variance of coefficient estimates, making them more sensitive to data variation.

At the same time, Figure 2, shows that the proposed three-quarter fold-over design exhibits lower correlation values than the semi-fold-over design. This observation indicates that, in the considered cases, the additional runs and fold-over construction help reduce the correlation between effects. As a result, the columns of the model matrix become less dependent, and the information matrix $X'X$ becomes closer to orthogonality. This is consistent with the role of fold-over designs in breaking alias chains and reducing confounding among effects (Montgomery, 2017).

It is worth noting that some level of multicollinearity is expected in such designs. As highlighted in optimal design theory (Atkinson, 2025), even when parameter estimates are correlated, a design can still achieve good predictive performance. In the present results, despite the observed correlation between effects (Figure 2), the proposed design maintains high D-efficiency and low APV. Therefore, the multicollinearity observed in the proposed design should be viewed as a consequence of the design structure rather than a major limitation.

Building on this observation, a noticeable effect is observed when two-factor interactions are selected for subsetting, particularly with respect to D-efficiency. This behavior can be explained by the structural impact of interaction-based selection on the design matrix. Specifically, two-factor interactions are more sensitive to the underlying alias structure in fractional factorial designs, and selecting them for subsetting tends to reduce orthogonality and introduce higher correlation among the columns of the design matrix. As a result, the information matrix becomes less stable, leading to a reduction in D-efficiency (Montgomery, 2017; Jones and Nachtsheim, 2011; Edwards & Mee, 2023).

In contrast, when subsetting is based on main effects, the impact on the design structure is relatively limited. Main effects are typically well-balanced and less affected by aliasing, which helps preserve design orthogonality. Consequently, subsetting based on main effects generally maintains a higher level of D-efficiency, although it may not capture the interaction structure within the design.

Despite these findings, this study has some limitations. The evaluation is based on a limited number of design examples, and the results may not generalize to all fractional factorial structures. In addition, only specific subsetting schemes were considered, and alternative choices may lead to different performance.

From a practical perspective, the proposed three-quarter fold-over design useful in situations where improved prediction accuracy is required without substantially increasing the number of experimental runs. This is supported by the results, in which the proposed

design achieves higher D-efficiency and lower APV than the initial and semi-fold-over designs. It can also serve as a practical alternative to full fold-over when experimental cost is a concern, particularly in follow-up experiments where partial de-aliasing is sufficient. Within the scope of the considered designs, the proposed design contributes to the literature on follow-up experimental designs by providing a flexible and efficient construction strategy.

Future work may extend the proposed three-quarter fold-over approach to other classes of designs, including nonorthogonal designs, with further attention to both construction and analysis aspects. In addition, exploring alternative subsetting strategies and their relationship with multicollinearity would be of interest. Evaluating the proposed designs using additional criteria, such as minimal dependent sets (MDS), also represents a promising direction for future research.

Overall, the proposed three-quarter fold-over design provides a practical and efficient solution for follow-up experimentation, offering a balance between estimation capability and experimental cost.

6. Declarations

The author declares that there are no competing interests.

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