

Optimal Semifoldover Plans for Two-Level Orthogonal Designs

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Abstract

Foldover is a widely used procedure for selecting follow-up experimental runs. As foldover designs require twice as many runs as the initial design, they can be inefficient if the number of effects to be dealiased is smaller than the size of the original experiment. Semifolding refers to adding half of a foldover fraction and is a technique that has been investigated in recent literature for regular two-level fractional factorial designs as an alternative to foldover. In this paper, a criterion for determining optimal semifoldover plans for two-level orthogonal factorial designs is proposed. Optimal plans are developed for selected 12, 16, 20, and 32-run designs and displayed for practical use. A hidden projection property of optimal semifoldovers of 12 and 20-run orthogonal arrays is also uncovered. General properties of semifoldover designs are obtained using indicator functions.

Keywords: Foldover, Generalized Minimum Aberration, Gröbner Bases, Indicator Function, Orthogonal Design, Semifoldover

1 Introduction and Motivation

Adding another fraction to an initial factorial design may be necessary in order to resolve ambiguities involving aliasing of effects in the initial experiment and/or to increase the precision of factorial effect estimates. Foldover is a classic technique used for selecting follow-up runs by reversing signs of one or more factors in the initial design. For instance,

it is well known that a full foldover (reversing the signs of all factor columns) of a resolution III design increases the resolution to IV and is often the optimal foldover plan. On the other hand, there can be numerous optimal foldover fractions for resolution IV designs (see Montgomery and Runger (1996)).

Li and Lin (2003) develop optimal foldover plans for two-level regular designs for run sizes of 16 and 32 with respect to the minimum aberration criterion of the combined design. Recall that *regular* fractional factorial designs are those that can be constructed using interaction contrasts to generate additional factors. Designs that do not possess this property are called *nonregular* (see Wu and Hamada (2000) for more). Instead, nonregular designs possess a more complex aliasing structure in that factorial effects may be partially aliased. Li et al. (2003) (henceforth, LLY) determine optimal foldover plans for two-level nonregular designs with 12, 16, and 20 runs based on the generalized minimum aberration (GMA) criterion of Deng and Tang (2002). They utilize the *indicator function* to study general properties of foldover designs.

Semifolding refers to adding half of a foldover fraction by subsetting on a factorial effect. Since a foldover design requires twice as many runs as the initial design, a semifoldover is a more efficient follow-up procedure. Mee and Peralta (2000) study semifolding for regular resolution IV designs and note that foldovers of 2_{IV}^{k-p} designs are often “degree of freedom inefficient” providing fewer than $n/2$ additional degrees of freedom for estimating two-factor interactions. They further discuss advantages of semifolding over D -optimal and Bayesian design augmentation strategies. See also John (2000). Lu and Lin (2006) address optimal semifoldover plans for regular resolution IV designs with 32-runs. In particular, they determine optimal semifoldovers by selecting subsetting factors such that the combined design is D -optimal among all choices. Furthermore, they show that a semifoldover plan determined by subsetting on a main effect, rather than a two or higher order interaction effect, can avoid multicollinearity among main effects and two-

factor interactions. Thus, only semifoldover plans based on subsetting a main effect will be investigated.

As motivation, consider the following example regarding a 2_{IV}^{10-5} with generators $X_6 = X_1X_2X_3X_4$, $X_7 = X_1X_2X_3X_5$, $X_8 = X_1X_2X_4X_5$, $X_9 = X_1X_3X_4X_5$, and $X_{10} = X_2X_3X_4X_5$. Li and Lin (2003) determine that an optimal foldover plan for this design is to reverse both factors X_6 and X_7 . Doing so produces a foldover design with the following aliasing structure (ignoring three and higher order interactions):

$$X_1X_{10} = X_2X_9 = X_3X_8,$$

$$X_1X_9 = X_2X_{10},$$

$$X_2X_8 = X_3X_9,$$

$$X_1X_8 = X_3X_{10},$$

$$X_4X_7 = X_5X_6,$$

$$X_4X_6 = X_5X_7,$$

$$X_4X_5 = X_6X_7,$$

$$X_2X_3 = X_8X_9,$$

$$X_1X_3 = X_8X_{10},$$

$$X_1X_2 = X_9X_{10}.$$

Using the criterion of Lu and Lin (2006), an optimal semifoldover plan is obtained by subsetting on *any* of the ten main effects. In Table 1, the aliasing of two-factor interactions for two semifoldover designs is shown. As can be seen, choosing to subset on X_4 permits the same partitioning of the two-factor interactions as does the full foldover. Clearly, this is a superior choice. From this example, it is observed that the D -optimality criterion is insufficient to determine an optimal semifoldover plan. In this article, a new criterion based on model estimability and GMA is proposed in order to find optimal semifoldovers for both regular and nonregular designs.

The remainder of this article proceeds as follows. In section 2, the basics of indica-

Table 1: Aliasing of Effects After Semifoldover of 2_{IV}^{10-5}

Subset on X_1	Subset on X_4
$X_1X_{10} = X_2X_9 = X_3X_8$	$X_1X_{10} = X_2X_9 = X_3X_8$
$X_1X_9 = X_2X_{10}$	$X_1X_9 = X_2X_{10}$
$X_2X_8 = X_3X_9$	$X_2X_8 = X_3X_9$
$X_1X_8 = X_3X_{10}$	$X_1X_8 = X_3X_{10}$
$X_4X_7 = X_5X_6$	$X_4X_7 = X_5X_6$
$X_4X_6 = X_5X_7$	$X_4X_6 = X_5X_7$
$X_4X_5 = X_6X_7$	$X_4X_5 = X_6X_7$
$X_2X_7 = -X_3X_5 + X_4X_9 + X_6X_8$	$X_2X_3 = X_8X_9$
$X_2X_5 = -X_3X_7 + X_4X_8 + X_6X_9$	$X_1X_3 = X_8X_{10}$
$X_2X_6 = -X_3X_4 + X_5X_9 + X_7X_8$	$X_1X_2 = X_9X_{10}$
$X_2X_4 = -X_3X_6 + X_5X_8 + X_7X_9$	
$X_2X_3 = X_8X_9$	
$X_1X_3 = X_8X_{10}$	
$X_1X_2 = X_9X_{10}$	

tor functions are reviewed. The use of algebraic geometry to solve model identifiability problems is also discussed. Section 3 discusses general properties of semifoldovers for orthogonal designs. Section 4 proposes a criterion to determine optimal semifoldover plans and presents results for selected 12, 16, 20, and 32-run designs. Section 5 is an analysis example of a semifoldover design and section 6 gives concluding remarks with suggestions for future research.

2 Indicator Functions, Word Length, and Gröbner Bases

Indicator functions are a useful mathematical tool that provide a way to characterize a factorial design by a polynomial whose coefficients reveal the aliasing of the design. The basics of indicator functions are now reviewed. For extensive details, see Fontana et al. (2000) and Ye (2003).

Consider an n -run fractional factorial design in k factors (denoted by \mathcal{D}). Then, \mathcal{D} is a finite set of distinct points in \mathbb{R}^k . The indicator function of \mathcal{D} (denoted by $F_{\mathcal{D}}$) is defined

such that

$$F_{\mathcal{D}}(x) = \begin{cases} r_x & \text{if } x \in \mathcal{D} \\ 0 & \text{if } x \in \mathbb{R}^k \setminus \mathcal{D} \end{cases} \quad (1)$$

where r_x is the number of replicates of the point x in \mathcal{D} . Define $X_{\ell}(x) = \prod_{i \in \ell} x_i$ for $\ell \in \mathcal{P}$, where \mathcal{P} is the collection of all subsets of $\{1, 2, \dots, k\}$. Then, the indicator function of \mathcal{D} has the following polynomial form:

$$F_{\mathcal{D}}(\mathbf{x}) = \sum_{\ell \in \mathcal{P}} b_{\ell} X_{\ell}(\mathbf{x}) \quad (2)$$

with coefficients

$$b_{\ell} = \frac{1}{2^k} \sum_{\mathbf{x} \in \mathcal{D}} X_{\ell}(\mathbf{x}). \quad (3)$$

For instance, $b_{\emptyset} = n/2^k$. It is straightforward to see that the coefficients, b_{ℓ} , are the signed J -characteristics (Deng and Tang (2002)) of \mathcal{D} up to a constant. For regular 2^{k-p} fractional factorial designs, the terms in the indicator function with nonzero coefficients are the *words* in the defining relation.

On the other hand, as a result of their complex aliasing structure, the indicator function is more complicated for nonregular designs. Consider the 16-run, 5-factor nonregular design given in Table 2. The polynomial form of its indicator function is

$$F(x_1, x_2, \dots, x_5) = \frac{1}{2^5} [16 + 8x_1x_4x_5 + 8x_2x_4x_5 + 8x_1x_3x_4x_5 - 8x_2x_3x_4x_5].$$

With the exception of the constant term, each term in the indicator function with a nonzero coefficient is called a *word*. LLY introduce the *generalized word length* as the number of letters in X_{ℓ} plus $(1 - |b_{\ell}/b_{\emptyset}|)$. For instance, the word $x_2x_4x_5$ in the above example has generalized word length of $3 + (1 - 8/16) = 3.5$. LLY further introduce the *extended word length pattern* (EWLP) of a design as $(f_1, \dots, f_{1+(n-1)/n}, f_2, \dots, f_{2+(n-1)/n}, \dots, f_k, \dots, f_{k+(n-1)/n})$,

Table 2: 16×5 nonregular design

X_1	X_2	X_3	X_4	X_5
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
-1	-1	-1	-1	1
-1	-1	-1	1	-1
-1	1	1	1	-1
-1	1	1	-1	1

where $f_{i+j/n}$ is the number of length- $(i + j/n)$ words in the indicator function. For the 16×5 nonregular design, we have $(f_{3.5} = 2, f_{4.5} = 2)$. Therefore, the *generalized resolution*, \mathcal{R} , is 3.5.

Pistone and Wynn (1996) introduce tools from algebraic geometry, in particular, Gröbner bases, to characterize the identifiable models of a design. In this article, these tools are utilized for both the design and analysis of semifoldover experiments. In particular, the Gröbner basis approach is useful as it guarantees a unique, estimable, and saturated model (M) for any design in however many factors. A review of their approach follows. For further details, see Giglio et al. (2000), Evangelaras and Koukouvinos (2006), Riccomagno (1997), and Holliday et al. (1999). For a book length treatment, see Pistone et al. (2001).

The key idea in the Gröbner basis approach is to represent a design by a system of polynomials whose solutions are the design points. The set of all polynomials in $\mathbb{R}[x_1, x_2, \dots, x_k]$ (i.e., the ring of all polynomials in k indeterminates with real coefficients) passing through the design points is called the *design ideal*. To compute a Gröbner basis for a design ideal,

one must first impose an *initial ordering* on the k factors. For instance, $x_1 \succ x_2 \succ \dots \succ x_k$. The choice of initial ordering should be made based on scientific knowledge or prior information, when available. One potential strategy for choosing an initial ordering is to fit a main effects only model and consider factor significance. Another suggestion is to apply forward selection and utilize the order in which variables are added to the model.

Aside from the initial ordering on the factors, one must also specify a *term ordering*, \succ_τ , on $\mathbb{R}^k[x_1, x_2, \dots, x_k]$. In particular, a term ordering is an order relation, \succ_τ , satisfying the following condition:

$$x_1^{\alpha_1} \dots x_k^{\alpha_k} \succ_\tau x_1^{\beta_1} \dots x_k^{\beta_k} \Rightarrow x_1^{\alpha_1 + \gamma_1} \dots x_k^{\alpha_k + \gamma_k} \succ_\tau x_1^{\beta_1 + \gamma_1} \dots x_k^{\beta_k + \gamma_k}$$

for all $(\alpha_1, \dots, \alpha_k)$, $(\beta_1, \dots, \beta_k)$, and $(\gamma_1, \dots, \gamma_k) \in \mathbb{Z}_+^k$. Two of the most widely used term orderings, pure lexicographical ordering and total degree ordering are now briefly mentioned.

The *pure lexicographical ordering*, \succ_{plex} , is given by

$$x_1^{\alpha_1} x_2^{\alpha_2} \dots x_k^{\alpha_k} \succ_{plex} x_1^{\beta_1} x_2^{\beta_2} \dots x_k^{\beta_k}$$

if and only if there exists an m such that $\alpha_1 = \beta_1, \dots, \alpha_{m-1} = \beta_{m-1}, \alpha_m > \beta_m$. This term ordering is akin to Yates order for factorial effects.

The *total degree ordering*, \succ_{tdeg} , is given by

$$x_1^{\alpha_1} x_2^{\alpha_2} \dots x_k^{\alpha_k} \succ_{tdeg} x_1^{\beta_1} x_2^{\beta_2} \dots x_k^{\beta_k}$$

if and only if $\sum_{i=1}^k \alpha_i > \sum_{i=1}^k \beta_i$ or $\sum_{i=1}^k \alpha_i = \sum_{i=1}^k \beta_i$ and there exists an m such that $\alpha_m < \beta_m, \alpha_{m+1} = \beta_{m+1}, \dots, \alpha_k = \beta_k$. That is, when the total degree ordering finds the same total degree, ties are broken in an inverse pure lexicographic order. The total degree ordering is both efficient for computation and reasonable for investigating models that assume a

hierarchical ordering as it favors lower order effects over higher order effects. Before defining a Gröbner basis, one more definition is in order.

For a polynomial $f \in \mathbb{R}[x_1, \dots, x_k]$, the *leading term* of f is that which is maximal with respect to τ among all terms in f . As an example, consider the polynomial $f(x_1, x_2, x_3) = 2x_1x_2^5x_3^2 + 3x_1^2x_2^3x_3^3 + 4x_1^3$ and an initial term ordering, $x_1 \succ x_2 \succ x_3$. Then, with respect to total degree ordering, we have $2x_1x_2^5x_3^2 \succ_{deg} 3x_1^2x_2^3x_3^3 \succ_{deg} 4x_1^3$ and thus $x_1x_2^5x_3^2$ is the leading term of f .

Given a term ordering, τ , a Gröbner basis, $\mathcal{G} = \{g_1(x), \dots, g_m(x)\}$, for a design ideal is a basis such that the solutions of $g_1, \dots, g_m = 0$ are the design points. Thus, the design ideal consists of all polynomials generated by \mathcal{G} (i.e. $\sum_{i=1}^n s_i(x)g_i(x)$ where $s_i(x)$ are polynomials). The set, M , of estimable effects is obtained as the set of terms not divisible by any of the leading terms of \mathcal{G} . Consider again the 16-run nonregular design in Table 2. Using Maple to perform computations, a Gröbner basis of this design with respect to total degree ordering and initial ordering $x_1 \succ x_2 \succ x_3 \succ x_4 \succ x_5$ is given by

$$\begin{aligned} \mathcal{G} = & \{x_1^2 - 1, x_2^2 - 1, x_3^2 - 1, x_4^2 - 1, x_5^2 - 1, 2x_4x_5 + x_2x_3 - x_1x_3 - x_2 - x_1, \\ & x_1x_2x_4 - x_2x_5 - x_1x_5 + x_4, x_1x_2x_5 - x_2x_4 - x_1x_4 + x_5, x_1x_3x_4 - x_3x_5 + x_1x_4 - x_5, \\ & x_1x_3x_5 - x_3x_4 + x_1x_5 - x_4, x_2x_3x_4 - x_3x_5 - x_2x_4 + x_5, x_2x_3x_5 - x_3x_4 - x_2x_5 + x_4\}. \end{aligned}$$

From this, we obtain

$$M = \{x_1, x_2, x_3, x_4, x_5, x_1x_2, x_1x_3, x_1x_4, x_1x_5, x_2x_3, x_2x_4, x_2x_5, x_3x_4, x_3x_5, x_2x_4x_5\}.$$

Thus, M consists of all main effects and two-factor interactions with the exception of x_4x_5 . In general, M presents the estimable effects that are more important than their aliased when considering the initial ordering. It can be shown that regardless of the initial ordering of the factors, 14 of the 15 available degrees of freedom are available to estimate main effects

and two-factor interactions.

3 Properties of Semifoldover Designs

Using the notation of LLY, denote a foldover plan by γ , where $X_i \in \gamma$ is a factor whose sign is reversed in the foldover design. Let \mathcal{D} be an n -run two-level design with indicator function $F_{\mathcal{D}}$ and let \mathcal{D}_{γ} be its foldover. The indicator functions of \mathcal{D}_{γ} and the combined design $\mathcal{D} \cup \mathcal{D}_{\gamma}$ are shown to be

$$F_{\mathcal{D}_{\gamma}} = F_{\mathcal{D}}((-1)^{\delta_1 x_1}, (-1)^{\delta_2 x_2}, \dots, (-1)^{\delta_k x_k}) \quad (4)$$

and

$$F_{\mathcal{D} \cup \mathcal{D}_{\gamma}} = F_{\mathcal{D}}(x_1, x_2, \dots, x_k) + F_{\mathcal{D}}((-1)^{\delta_1 x_1}, (-1)^{\delta_2 x_2}, \dots, (-1)^{\delta_k x_k}) \quad (5)$$

where $\delta_i=1$ if $X_i \in \gamma$ and 0 otherwise ($i = 1, 2, \dots, k$). Some general properties of semifoldover designs are now developed with proofs provided in the appendix. As noted before, only semifoldovers based on subsetting a single factor are considered.

Proposition 3.1. *Let $S_{\mathcal{D}}^{X_i}$ be any $n/2$ treatment combinations of a two-level design, \mathcal{D} , such that a single factor, X_i , has common sign $\alpha = +1$ or -1 . Then, the indicator function of $S_{\mathcal{D}}^{X_i}$ is given by $F_{S_{\mathcal{D}}^{X_i}} = \frac{1+(-1)^{\omega x_i}}{2} F_{\mathcal{D}}$ where $\omega = \begin{cases} 1 & \text{if } \alpha = -1 \\ 0 & \text{if } \alpha = 1 \end{cases}$.*

It immediately follows from Proposition 3.1 that the indicator functions of the semifold fraction, $S_{\mathcal{D}_{\gamma}}^{X_i}$, and the combined design $\mathcal{D} \cup S_{\mathcal{D}_{\gamma}}^{X_i}$ are given by

$$F_{S_{\mathcal{D}_{\gamma}}^{X_i}} = \frac{1+(-1)^{\omega x_i}}{2} F_{\mathcal{D}}((-1)^{\delta_1 x_1}, (-1)^{\delta_2 x_2}, \dots, (-1)^{\delta_k x_k}) \quad (6)$$

and

$$F_{\mathcal{D} \cup S_{\mathcal{D}_\gamma}^{X_i}} = F_{\mathcal{D}}(x_1, x_2, \dots, x_k) + \frac{1 + (-1)^{\omega x_i}}{2} F_{\mathcal{D}}((-1)^{\delta_1 x_1}, (-1)^{\delta_2 x_2}, \dots, (-1)^{\delta_k x_k}) \quad (7)$$

where δ_i and ω are defined as before.

Proposition 3.2. *Let \mathcal{A} be a two-level orthogonal array with $3 \leq \mathcal{R}_{\mathcal{A}} < 4$ and $S_{\mathcal{A}_\gamma}^{X_i}$ be a semifold fraction of \mathcal{A} constructed by subsetting on X_i with common sign α and where $\gamma = \{X_1, X_2, \dots, X_k\}$. Then, the combined design $\mathcal{A} \cup S_{\mathcal{A}_\gamma}^{X_i}$ dealiases X_i from its two-factor interaction aliases.*

Propositions 3.3 and 3.4 are generalizations of results given by Mee and Peralta (2000) and Mee and Xiao (2008) to two-level orthogonal designs.

Proposition 3.3. *Let \mathcal{B} be a two-level orthogonal array with generalized resolution $4 \leq \mathcal{R}_{\mathcal{B}} < 5$ and $S_{\mathcal{B}_\gamma}^{X_i}$ be a semifold fraction of \mathcal{B} constructed by subsetting on X_i and where γ consists of a single factor. Then, the combined design $(\mathcal{B} \cup S_{\mathcal{B}_\gamma}^{X_i})$ permits estimation of the same two-factor interactions as the foldover design $(\mathcal{B} \cup \mathcal{B}_\gamma)$ assuming three-factor and higher order interactions are negligible.*

Before stating Proposition 3.4, note that a two-level orthogonal array is defined to be even if its indicator function only contains words with an even number of letters.

Proposition 3.4. *Let \mathcal{E} be an even orthogonal array with generalized resolution $4 \leq \mathcal{R}_{\mathcal{E}} < 5$ and let \mathcal{E}_γ be any $n \times k$ foldover fraction of \mathcal{E} . Then a semifold design $(\mathcal{E} \cup S_{\mathcal{E}_\gamma}^{X_i})$ constructed by subsetting on X_i , can estimate the same number of two-factor interactions as the foldover design $(\mathcal{E} \cup \mathcal{E}_\gamma)$ assuming three-factor and higher order interactions are negligible.*

4 Optimal Semifoldover Plans

In this section, optimal semifolder plans for orthogonal designs are discussed. Recall that LLY utilize the GMA criterion in order to search for optimal folder designs. In particular, for the combined design $\mathcal{D} \cup \mathcal{D}_\gamma$, an optimal folder is given by γ^* such that $\text{EWLP}(\mathcal{D} \cup \mathcal{D}_{\gamma^*}) = \min_\gamma \text{EWLP}(\mathcal{D} \cup \mathcal{D}_\gamma)$. That is, the optimal folder is that which sequentially minimizes the number of words in the EWLP that are of minimum length.

The aforementioned criterion can similarly be utilized in determining optimal semifolders. Denote an optimal semifolder plan as (γ^*, X_i^*) . Having already determined an optimal folder, γ^* , one seeks a semifolder design such that

$$\text{EWLP}(\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_{\gamma^*}}^{X_i^*}) = \min_{X_i \in \mathcal{X}} \text{EWLP}(\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_{\gamma^*}}^{X_i}) \quad (8)$$

where \mathcal{X} represents the set of factors that are candidates for subsetting. Unfortunately, use of GMA alone is not a sufficient criterion. Reconsider the 2_{IV}^{10-5} illustrated in section 1 in which it was shown that a particular semifolder design was superior to another. Since all semifolder designs possess identical EWLPs in this example, any distinction with GMA is impossible.

As discussed in section 2, the Gröbner basis approach allows one to identify a saturated set of estimable terms, $M_{\mathcal{D}}$, for any design, \mathcal{D} . For use in determining an optimal semifolder plan, let us specify only main effects and two-factor interactions as those terms of interest. Then, for any semifolder design, $\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_\gamma}^{X_i}$, the set $M_{\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_\gamma}^{X_i}}$, while not necessarily saturated, contains the main effects and two-factor interactions which are not divisible by the leading terms of the Gröbner basis, \mathcal{G} . Certainly, a semifolder plan that can estimate as many main effects and two-factor interactions as possible is desirable. Thus, the cardinality of $M_{\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_\gamma}^{X_i}}$, denoted as $\left| M_{\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_\gamma}^{X_i}} \right|$, should be maximized. Of course, one could simply determine the identifiability of a specific model by noting the rank of the model

matrix. The Gröbner basis approach is more revealing, though, as the set $M_{\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_\gamma}^{X_i}}$ is useful in the analysis of the combined design (which is an irregular fraction). An example is presented in section 5. Since the primary objective of semifolding is to estimate more effects while saving experimental runs, a criterion should first maximize $\left| M_{\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_\gamma}^{X_i}} \right|$.

Thus, a criterion for determining an optimal semifoldover plan is now proposed:

1. Find an optimal foldover plan, γ^* , using the methods of LLY.
2. From all factors, $\{X_i, i = 1, \dots, k\}$, determine the set of subsetting candidates, \mathcal{X} , such that $\mathcal{X} = \max_{\{X_i, i=1, \dots, k\}} \left| M_{\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_{\gamma^*}}^{X_i}} \right|$.
3. For a given design, \mathcal{D} , an optimal semifoldover plan is given by (γ^*, X_i^*) such that $\text{EWLP}(\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_{\gamma^*}}^{X_i^*}) = \min_{X_i \in \mathcal{X}} \text{EWLP}(\mathcal{D} \cup \mathcal{S}_{\mathcal{D}_{\gamma^*}}^{X_i})$.

In what follows, the proposed criterion is utilized to determine optimal semifoldover plans for both regular and nonregular designs of various run sizes. While an attempt is not made to construct a complete catalog except for the case of 32-run regular resolution IV designs, optimal semifoldover plans for designs not shown can be easily determined in a similar manner.

Tables 5-14 of LLY provide optimal foldover plans for all nonisomorphic 16-run designs. Using their recommended foldover plans, Table 3 provides optimal semifoldover plans for selected 16-run designs with $k \geq 5$. The initial design coding is based on the catalog of Deng and Tang (2002). As the results will be used subsequently, optimal semifoldover plans for all nonisomorphic 16×5 designs are given.

Table 4 provides a complete catalog of optimal semifoldover plans for regular resolution IV designs with 32-runs. Here, the initial design coding is based on Chen et al. (1993). These results extend those of Lu and Lin (2006), who only provide results up to $k = 11$. An asterisk (*) denotes an optimal semifoldover plan that differs from their findings.

Tables 5 and 6 summarize optimal semifoldover plans for selected 12 and 20-run orthogonal arrays, respectively, for $k \geq 5$. Results for all nonisomorphic designs with $k=5$ are provided. The initial design coding in Table 6 is based on the catalog of Deng and Tang (2002). Given that the optimal foldover plan for 12 and 20-run two-level orthogonal arrays is the full foldover plan (see LLY), the foldover plan column is omitted from Tables 5 and 6.

Diamond (1995) showed that projecting the full foldover of a 12-run Plackett-Burman design on to any five factors allows for estimation of all main effects and two-factor interactions. Cheng (1998) proves that this *hidden projection property* holds for any orthogonal array with generalized resolution, $4 \leq \mathcal{R} < 5$, and whose run size is not a multiple of 16. Based on the cardinality of M in Tables 3, 5, and 6 for $k=5$, one can discover the following result, which extends the findings of Diamond (1995) and partially those of Cheng (1998) to semifoldover designs.

Result 4.1. *Let \mathcal{D} be a 12 or 20-run orthogonal array. Assume that all three-factor and higher-order interactions are negligible. Then, all main effects and two-factor interactions are estimable in the projection of an optimal semifoldover design $(\mathcal{D} \cup S_{\mathcal{D}_\gamma^*}^{X_i^*})$ on to any five factors.*

Based on results not shown, Result 4.1 can be strengthened for 12-run OAs to state that all main effects and two-factor interactions are estimable in the projection of *any* semifoldover plan (based on subsetting a main effect) on to any five factors. Although many five factor projections of an optimal semifoldover of 16-run designs may permit estimation of all main effects and two-factor interactions, Table 3 demonstrates that an analogous result to 4.1 does not hold.

Table 3: Optimal Semifoldover Plans for Selected $16 \times k$ Designs

k	Initial Design	Foldover Plan (γ)	Optimal Semifold Factors	\mathcal{M}
5	16.5.1	1	1,2,3,4,5	15
5	16.5.2	1	1,2,3,4,5	15
5	16.5.3	3	2	15
5	16.5.4	4	3,4	15
5	16.5.5	4	1,2,3	15
5	16.5.6	5	1,2,4,5	15
5	16.5.7	1,2	2	15
5	16.5.8	5	5	15
5	16.5.9	1	3,5	15
5	16.5.10	1,4	4,5	14
5	16.5.11	1	2,3,4,5	11
6	16.6.1	1	1,2,3,4,5,6	18
6	16.6.2	1,5	3,4	18
6	16.6.3	6	5,6	20
7	16.7.1	1,6	1,2,3,4,5,6,7	20
7	16.7.2	1,7	4,5	23
7	16.7.3	2,3,4	2,3,4	23
8	16.8.1	1,2	1,2,3,4,5,6,7,8	21
8	16.8.2	1,3,4	3,4,5,6,7,8	23
8	16.8.3	2,3,4	2,3,4	23
9	16.9.1	9	4,5,6,7	23
9	16.9.2	1,2,3,4	1,2	23
9	16.9.3	1,2,3,4	2	23
10	16.10.1	1,2,3,4	9,10	23
10	16.10.2	1,2,3,4	5,6,7,8,9,10	23
10	16.10.3	9,10	9,10	23
11	16.11.1	1,2,3,4	7	23
11	16.11.2	full foldover	10,11	23
11	16.11.3	1,2,3,4	10,11	23
12	16.12.1	1,2,3,4	5,6,7,8,9,10,11,12	23
12	16.12.2	1,2,3,4	5,6,7,8,9,10,11,12	23
12	16.12.3	1,2,3,4	1,2,3,4,5,6,7,8,10,11,12	23
13	16.13.1	full foldover	2,3,4,5,6,7,8,9,10,11,12,13	23
13	16.13.2	1,2,3,4,5	6,7,8,9,10,11,12,13	23
13	16.13.3	1,2,3,4	6,7,8,9,10,11,12,13	23
14	16.14.1	full foldover	1,2,3,4,5,6,7,8,9,10,11,12,13,14	23
14	16.14.2	1,2,3,4,5,6	7,8,9,10,11,12,13,14	23
14	16.14.3	1,2,3,4,5,6	7,8,9,10,11,12,13,14	23

Table 4: Optimal Semifoldover Plans for 32-run FFDs of Resolution IV

k	Initial Design	Foldover Plan (γ)	Optimal Semifold Factors	\mathcal{M}
7	7-2.1	6	1,2,4	28
7	7-2.2	6,7	2,3,4,5,6,7	28
7	7-2.3	6,7	5	25
8	8-3.1	6,7,8	5,8	33
8	8-3.2	7,8	4,5,7,8	33
8	8-3.3	6,7	1,2,3,4,5,6,7,8*	30
8	8-3.4	6	5	28
9	9-4.1	6,7	5	39
9	9-4.2	6,7	5,9	37
9	9-4.3	7,8	1,2,3,4,5,6,7,8,9	36
9	9-4.4	8,9	5,9	37
9	9-4.5	6,7	5	30
10	10-5.1	6,7	4,5,6,7*	44
10	10-5.2	6,7,8	1,2,3,4,5,6,7,8,9	40
10	10-5.3	8,9	4,5,7,8,9,10*	39
10	10-5.4	8,9,10	4,5,7,8,9,10*	39
11	11-6.1	6,8,9	2,3,4,5,6,7,8,9,10,11*	41
11	11-6.2	8,9,10	5,10,11*	41
12	12-7.1	6,7,11	5,10,11,12	42
12	12-7.2	7,8,10,12	1,2,3,4,5,6,7,8,9,10,11,12	42
13	13-8.1	7,8,10,12	13	43
14	14-9.1	6,7,11,14	1,2,3,4,5,6,7,8,9,10,11,12,13,14	44
15	15-10.1	6,7,11,14,15	1,2,3,4,5,6,7,8,9,10,11,12,13,14,15	45
16	16-11.1	6,7,8,9,10,15	1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16	46

Table 5: Optimal Semifoldover Plans for the 12-run Plackett-Burman Design

k	Initial Design	Optimal Semifold Factors	\mathcal{M}
5	5.1	1,2,3,4,5	15
5	5.2	1,2,3,4,5	15
6	6.1	3,6	17
6	6.2	3,6	17
7	7.1	1,3,4,5,6,7	17
8	8.1	1,6,8	17
9	9.1	1,2,3,4,5,6,7,8,9	17
10	10.1	1,2,3,4,5,6,7,8,9,10	17
11	11.1	1,2,3,4,5,6,7,8,9,10,11	17

Table 6: Optimal Semifoldover Plans for selected $20 \times k$ Designs

k	Initial Design	Optimal Semifold Factors	\mathcal{M}
5	20.5.1	1,2,3,4,5	15
5	20.5.2	2	15
5	20.5.3	5	15
5	20.5.4	3	15
5	20.5.5	1	15
5	20.5.6	2,4	15
5	20.5.7	3,4	15
5	20.5.8	2,3	15
5	20.5.9	1,2	15
5	20.5.10	1,2,3	15
6	20.6.1	3	20
6	20.6.2	4	21
6	20.6.3	3	20
7	20.7.1	3,5	24
7	20.7.2	2	25
7	20.7.3	2	23
8	20.8.1	5,6,7,8	27
8	20.8.2	4,5	25
8	20.8.3	2,8	25
9	20.9.1	1,2,3,8,9	27
9	20.9.2	1,2,3,8,9	27
9	20.9.3	3	27
10	20.10.1	8	29
10	20.10.2	4	29
10	20.10.3	1	28
11	20.11.1	2,3,10,11	29
11	20.11.2	8,9	29
11	20.11.3	10	29
12	20.12.1	9,10,11,12	29
12	20.12.2	6	29
12	20.12.3	1	29
13	20.13.1	12,13	29
13	20.13.2	10,11,12,13	29
13	20.13.3	3,5,10	29
14	20.14.1	1	29
14	20.14.2	11,12,13,14	29
14	20.14.3	11,14	29
15	20.15.1	8	29
15	20.15.2	13	29
15	20.15.3	5,7	29
16	20.16.1	5,9	29
16	20.16.2	14	29

5 Analysis Example

Miller and Sitter (2001) present the results of a nine-factor experiment that investigated ways of reducing the level of a toxic contaminant from the waste stream of a chemical operation using the full foldover of a 12-run Plackett-Burman design. Suppose, however, that conducting 24 experimental runs was deemed too expensive. Based on Table 5, an optimal semifoldover design can be constructed by subsetting on any of the nine main effects. An 18-run semifoldover design obtained by subsetting on the high level of factor A is shown in Table 7.

In order to apply the Gröbner basis approach to analysis, it is necessary to first impose an initial ordering on the factors. Based on an earlier suggestion, a main-effects only model is fit to the data and the order of factor significance is utilized to determine the initial ordering. In doing so (results not shown), we have $B \succ A \succ G \succ I \succ C \succ F \succ E \succ D \succ H$. After obtaining a Gröbner basis for the design with respect to total degree ordering, we find

$$M = \{A, B, C, D, E, F, G, H, I, AB, AG, BC, BE, BF, BG, BH, BI\}.$$

A normal plot of these 17 effects is shown in Figure 1 and indicates that only A , B , and the AB interaction are significant. Fitting a model with only these three terms produces $R^2=0.9999$, indicating a very good fit. These results are consistent with those obtained in Miller and Sitter (2001). Certainly, the Gröbner basis approach provides a useful alternative to current methods for analyzing designs with complex aliasing (see, for instance, Hamada and Wu (1992) and Chipman et al. (1997)).

6 Concluding Remarks

In this article, optimal semifoldover plans for two-level orthogonal designs have been investigated. Indicator functions are utilized to prove several general properties of semifoldover

Table 7: Semifoldover Design Based on Contamination Data from Miller and Sitter (2001)

<i>A</i>	<i>B</i>	<i>C</i>	<i>D</i>	<i>E</i>	<i>F</i>	<i>G</i>	<i>H</i>	<i>I</i>	Contaminant
1	1	-1	1	1	1	-1	-1	-1	1.3
1	-1	1	1	1	-1	-1	-1	1	790.3
-1	1	1	1	-1	-1	-1	1	-1	5.74
1	1	1	-1	-1	-1	1	-1	1	12.6
1	1	-1	-1	-1	1	-1	1	1	7.38
1	-1	-1	-1	1	-1	1	1	-1	799.01
-1	-1	-1	1	-1	1	1	-1	1	324.78
-1	-1	1	-1	1	1	-1	1	1	341.33
-1	1	-1	1	1	-1	1	1	1	5.54
1	-1	1	1	-1	1	1	1	-1	795.47
-1	1	1	-1	1	1	1	-1	-1	3.68
-1	-1	-1	-1	-1	-1	-1	-1	-1	326.37
1	-1	-1	-1	1	1	1	-1	1	789.95
1	1	1	-1	1	-1	-1	1	-1	5.33
1	1	-1	1	-1	-1	1	-1	-1	8.78
1	-1	1	-1	-1	1	-1	-1	-1	798.49
1	-1	-1	1	-1	-1	-1	1	1	792.02
1	1	1	1	1	1	1	1	1	7.89

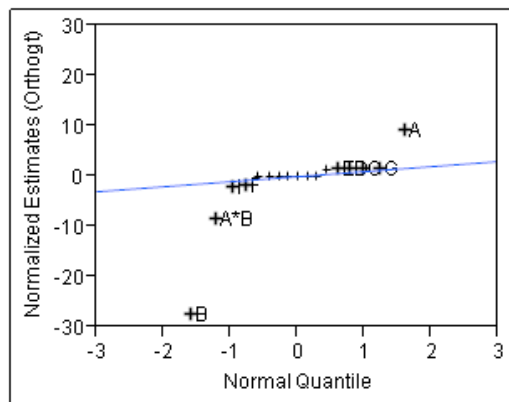


Figure 1: Normal Plot of Effects for Contaminant Data

plans. Optimal plans are provided for selected 12, 16, 20, and 32-run designs. It was shown that the GMA criterion is alone not sufficient for finding an optimal semifoldover. Thus, in conjunction with GMA, tools from algebraic geometry (in particular, Gröbner bases) were presented as a means of determining optimal semifoldover plans that provide for maximal estimation of effects. Although able to provide one with a saturated identifiable model, Gröbner bases were used as a means of uncovering the estimable main effects and two-factor interactions for a given semifold design. It is seen that an optimal semifoldover plan allows for estimation of all main effects and two-factor interactions for any five factor projection of 12 and 20-run orthogonal arrays.

Aside from its use in developing a design criterion, the Gröbner basis approach is instructive for analysis of semifoldover designs as shown in section 5. Clearly, the aliasing of effects does not necessarily allow for estimation of all effects of interest even if enough degrees of freedom are available. Since in practice an experimenter does not know if the saturated model they can potentially identify consists of all main effects, two-factor interactions, and then higher-order interactions, Gröbner bases provide a useful method for determining an efficient saturated model amidst aliasing.

Miller and Sitter (2005) discuss foldovers of nonorthogonal designs and their use in screening applications. Lin et al. (2008) introduce a criterion to compare foldovers of nonorthogonal designs. Such ranking and comparison of nonorthogonal designs could likewise be performed using the criterion of section 4. Future research should also consider optimal design and analysis of semifoldover plans for nonorthogonal designs. This potentially worthy topic has yet to be explored. By specifying a saturated estimable model for any design, the Gröbner basis approach can easily help simplify the sometimes daunting task of analyzing nonorthogonal designs.

Appendix: Proofs of Propositions

Proof of Proposition 3.1

Let \mathcal{L} be the set of words in the indicator function $F_{\mathcal{D}}$. Clearly, any word in $F_{\mathcal{D}}$ (i.e. $X_\ell \in \mathcal{L}$) will remain in $F_{S_{\mathcal{D}}^{X_i}}$, but with coefficients of $b_\ell/2$. By subsetting on X_i , $F_{S_{\mathcal{D}}^{X_i}}$ will also contain words of the form $(-1)^{\omega_{X_i} X_\ell}$ with coefficients $b_\ell/2$. Thus, $F_{S_{\mathcal{D}}^{X_i}} = \frac{1}{2}F_{\mathcal{D}} + \frac{1}{2}(-1)^{\omega_{X_i}}F_{\mathcal{D}} = \frac{1+(-1)^{\omega_{X_i}}}{2}F_{\mathcal{D}}$ as desired. \square

Proof of Proposition 3.2

Since $3 \leq \mathcal{R}_{\mathcal{A}} < 4$, $F_{\mathcal{A}}$ contains words with three or more letters. Combining $S_{\mathcal{A}_\gamma}^{X_i}$ with the treatment combinations in \mathcal{A} in which $X_i = \alpha$ (denote this as $S_{\mathcal{A}}^{X_i}$), we have

$$F_{S_{\mathcal{A}}^{X_i} \cup S_{\mathcal{A}_\gamma}^{X_i}}(x_1, \dots, x_i, \dots, x_k) = \frac{1 + (-1)^{\omega_{X_i}}}{2} \left[F_{\mathcal{A}}(x_1, \dots, x_i, \dots, x_k) + F_{\mathcal{A}_\gamma}(-x_1, \dots, -x_i, \dots, -x_k) \right].$$

Then, $F_{S_{\mathcal{A}}^{X_i} \cup S_{\mathcal{A}_\gamma}^{X_i}}$ does not possess any three letter words containing X_i . Thus, X_i is dealiased from its two-factor interaction aliases. \square

Proof of Proposition 3.3

Case 1. Suppose $\gamma = \{X_i\}$ and $S_{\mathcal{B}_\gamma}^{X_i}$ is constructed by subsetting on X_i . Since, $4 \leq \mathcal{R}_{\mathcal{B}} < 5$, $F_{\mathcal{B}}$ contains words with four or more letters. Then, combining $S_{\mathcal{B}_\gamma}^{X_i}$ with the treatment combinations in \mathcal{B} in which $X_i = \alpha$ (denoted by $S_{\mathcal{B}}^{X_i}$), we have

$$F_{S_{\mathcal{B}}^{X_i} \cup S_{\mathcal{B}_\gamma}^{X_i}}(x_1, \dots, x_i, \dots, x_k) = \frac{1 + (-1)^{\omega_{X_i}}}{2} \left[F_{\mathcal{B}}(x_1, \dots, x_i, \dots, x_k) + F_{\mathcal{B}_\gamma}(x_1, \dots, -x_i, \dots, x_k) \right].$$

Then, $F_{S_{\mathcal{B}}^{X_i} \cup S_{\mathcal{B}_\gamma}^{X_i}}$ does not contain any four letter words with X_i . Furthermore, $F_{S_{\mathcal{B}}^{X_i} \cup S_{\mathcal{B}_\gamma}^{X_i}}$ only contains words with four or more letters with the exception of the word x_i . Thus, $X_j + X_i X_j$ ($i \neq j$) is estimable from $S_{\mathcal{B}}^{X_i} \cup S_{\mathcal{B}_\gamma}^{X_i}$. Since each main effect is estimable from \mathcal{B} , it follows

that each $X_i X_j$ is estimable from $\mathcal{B} \cup \mathcal{S}_{\mathcal{B}_\gamma}^{X_i}$.

Case 2. Suppose $\gamma = \{X_i\}$ and $\mathcal{S}_{\mathcal{B}_\gamma}^{X_j}$ is constructed by subsetting on X_j ($i \neq j$). Then, combining $\mathcal{S}_{\mathcal{B}_\gamma}^{X_j}$ with the treatment combinations in \mathcal{B} in which $X_j = \alpha$ we have

$$F_{\mathcal{S}_{\mathcal{B}}^{X_j} \cup \mathcal{S}_{\mathcal{B}_\gamma}^{X_j}}(x_1, \dots, x_i, \dots, x_k) = \frac{1 + (-1)^{\omega} x_j}{2} \left[F_{\mathcal{B}}(x_1, \dots, x_i, \dots, x_k) + F_{\mathcal{B}_\gamma}(x_1, \dots, -x_i, \dots, x_k) \right].$$

Then, $F_{\mathcal{S}_{\mathcal{B}}^{X_j} \cup \mathcal{S}_{\mathcal{B}_\gamma}^{X_j}}$ has no word containing X_i . Furthermore, $F_{\mathcal{S}_{\mathcal{B}}^{X_j} \cup \mathcal{S}_{\mathcal{B}_\gamma}^{X_j}}$ only consists of words with three or more letters with the exception of x_j . Therefore, $X_i + X_i X_j$ is estimable from $\mathcal{S}_{\mathcal{B}}^{X_j} \cup \mathcal{S}_{\mathcal{B}_\gamma}^{X_j}$ as well as $X_i X_{i'}$ for $i' \neq j$. Since each main effect is estimable from \mathcal{B} , $X_i X_j$ is estimable from $\mathcal{B} \cup \mathcal{S}_{\mathcal{B}_\gamma}^{X_j}$. \square

Lemma A.1. *An n -run two-level even design must be a full foldover design. That is, it can be partitioned as C , followed by the full foldover $-C$, where C is $n/2 \times k$.*

Proof. See Cheng et al. (2008) \square

Proof of Proposition 3.4

Let $\mathbf{X}(\mathcal{E}) = [\mathbf{X}_1(\mathcal{E}) \ \mathbf{X}_2(\mathcal{E})]$ where $\mathbf{X}_1(\mathcal{E}) = [\mathbf{1} \ \mathcal{E}]$ ($\mathbf{1}$ is a column of 1's) and $\mathbf{X}_2(\mathcal{E})$ is the $n \times k(k-1)/2$ matrix of two-factor interactions based on taking all pairwise products of the columns of \mathcal{E} . Since \mathcal{E} is even, \mathcal{E}_γ is also an even design. Therefore, by Lemma A.1, \mathcal{E}_γ can be partitioned as

$$\begin{bmatrix} C \\ -C \end{bmatrix}$$

where C is $n/2 \times k$. Denote the $n/2 \times k$ semifold fraction based on subsetting on X_i by $\mathcal{S}_{\mathcal{E}_\gamma}^{X_i}$.

It is straightforward to see that by rearranging the rows of \mathcal{B}_γ , we have $\mathcal{S}_{\mathcal{E}_\gamma}^{X_i} = C$. Thus,

$$\text{rank}(\mathbf{X}_2(\mathcal{E}_\gamma)) = \text{rank}\left(\mathbf{X}_2\left(\begin{bmatrix} C \\ -C \end{bmatrix}\right)\right) = \text{rank}(\mathbf{X}_2(C)) = \text{rank}(\mathbf{X}_2(\mathcal{S}_{\mathcal{E}_\gamma}^{X_i})).$$

Therefore,

$$\text{rank}(\mathbf{X}_2(\mathcal{E} \cup \mathcal{E}_\gamma)) = \text{rank}(\mathbf{X}_2(\mathcal{E} \cup \mathcal{S}_{\mathcal{E}_\gamma}^{X_i})). \square$$

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