Geometric aliasing, Generalized defining relations, and Gröbner basis: A New Look at Multi-level Factorial Designs

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Multi-level factorial designs are useful in experiments but their aliasing structure are complex compare to two-level fractional factorial designs. A new framework is proposed to study the complex aliasing of those designs. Geometric aliasing is defined for factorial designs. It generalize of the aliasing relation of regular two level fractional factorial designs to all factorial designs. Based on geometric aliasing, generalized defining relations are defined for a large group of factorial designs. They determine the complete geometric aliasing structure of a design. The mathematical tools for studying geometric aliasing are available in computational algebraic geometry. Two examples are presented to show how this methodology can be used to reveals structure of factorial designs.

KEY WORDS: Experimental design, Orthogonal arrays, Confounding, Contrasts, Polynomial models, Computational algebraic geometry, Algebraic variety

1 INTRODUCTION

Multi-level factorial designs such as three-level factorial designs, and mixed level factorial designs are popular in industrial experiments. Unlike two-level fractional factorial designs, their aliasing structure are complicated and cannot be easily derived. For three-level fractional factorial designs, the aliasing structure derived from their defining relations is in a pure combinatorial sense and does not have the same nice interpretation as in the two-level design. Moreover, there are no defining relations for mixed level factorial designs and there is no general method for studying their aliasing structure. In this paper, I propose a new framework for studying aliasing structures of multi-level factorial designs.

Consider a 3^{4-2} fractional factorial design listed in Table 1. It has four factors and is generated by defining relations $C = AB$ and $D = AB^2$. To analyze the data, one could fit the response of this experiment with a polynomial model of their main contrasts as suggested in Wu and Hamada (2000). The two degrees of freedom for each factor in the 3^{4-2} design can be decomposed into linear and quadratic components. Let y_0, y_1, y_2 represent the observations at level 0, 1 and 2 of factor A. The linear effect and

Table 1: 3^{4-2} fractional factorial design

A	B	C	D
0	0	0	0
0	1	1	2
0	2	2	1
1	0	1	1
1	1	2	0
1	2	0	2
2	0	2	2
2	1	0	1
2	2	1	0

quadratic effect are defined as $y_2 - y_0$ and $y_0 + y_2 - 2y_1$ respectively. Mathematically, the two effects are obtained by taking the inner product of vector $y = (y_0, y_1, y_2)$ and $A_l = \frac{1}{\sqrt{2}}(-1, 0, 1)$, $A_q = \frac{1}{\sqrt{6}}(1, -2, 1)$ respectively. A_l and A_q are called main effect contrasts that define linear and quadratic effects. Similarly, we can define contrasts B_l, B_q, C_l, C_q, D_l, and D_q. The contrast matrix which contains all eight contrasts is shown in Table 2. The interactions of two factors can be decomposed into four components. The contrast of linear-linear interaction of A and B is defined as A_lB_l, Shur product of vectors A_l and B_l. Linear-quadratic, quadratic-linear and quadratic-quadratic component of AB interaction are similarly defined. Wu and Hamada (2000) also gives nice interpretation of these interaction contrasts. It is easy to verify that all four components are orthogonal. We call this decomposition a linear-quadratic system. In general, similar decomposition can be applied to any factorial designs

Table 2: Contrast Matrix of 3^{4-2} fractional factorial design

A_l	A_q	B_l	B_q	C_l	C_q	D_l	D_q
-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	0	2	0	2	1	-1
-1	-1	1	-1	1	-1	0	2
0	2	-1	-1	0	2	0	2
0	2	0	2	1	-1	-1	-1
0	2	1	-1	-1	-1	1	-1
1	-1	-1	-1	1	-1	1	-1
1	-1	0	2	-1	-1	0	2
1	-1	1	-1	0	2	-1	-1

with multiple levels. To analyze the result of such experiments, the responses can be fitted by linear models in which main effect contrasts and two-factor interaction contrasts are predictors. To choose an efficient design, it is important to understand the aliasing relations among contrasts of a factorial design. The traditional aliasing relations of the 3^{4-2} derived from its defining relations $C = AB$ and $D = AB^2$, however, are in a combinatorial sense. They give little information about fitting polynomial response surface models under the linear-quadratic system. Therefore, an alternative aliasing relations need to be defined to deal with the aliasing of predictors in the polynomial model.

Definition 1 *Predictors $X_1, X_2, \cdots, X_p$ are said to be geometrically aliased if they are linearly dependent. Particularly, contrasts associated with an factorial design are said to be geometrically aliased if they are linearly dependent.*

In their pioneering paper, Pistone and Wynn (1996) introduce the idea of using algebraic geometry theory into experimental design. They show that "generalized confounding" of a design can be studied using algebraic geometry. The connection between algebraic geometry and experimental design is briefly presented in Section 2. Section 3 defines the generalized defining relation and shows that they can be obtained by the Gröbner basis method. Section 4 gives two examples to illustrate how the new method helps in designing experiments and analyzing data.

2 ALGEBRAIC GEOMETRY AND GRÖBNER BASIS

In this section, I will briefly explain Gröbner basis, which is part of a well established theory of computational algebraic geometry. Here, I will only cover a tiny portion of the theory that is relevant. For more on computational algebraic geometry, I will refer to Cox, Little and O'Shea (1997).

First, a contrast matrix of d variables of a design, is a set of points in R^d. In algebraic geometry, it is called a variety. Let $I(V)$ be the collection of all polynomials that have zeros on a variety V. That is, all these polynomials vanish on all design points. Based on the definition of geometric aliasing, the terms of a polynomial in $I(V)$ are geometrically aliased since they are linearly dependent. In other words, a linear model containing all those terms are not estimable. It can be easily seen that $I(V)$

has following two properties:

(i) For $f, g \in I(V)$, $f + g \in I(V)$;

(ii) For $f \in I(V)$, h be any polynomial, $fh \in I(V)$.

Following the definition of ideal, $I(V)$ is an ideal in a polynomial ring.

One of the most important theorem regarding ideals in a polynomial ring is Hilbert Basis Theorem.

Theorem 2 (Hilbert Basis Theorem). *Every ideal $I \subset k[x_1, x_2, \cdots, x_d]$ has a finite generating set, where $k[x_1, x_2, \cdots, x_d]$ is the polynomial ring with d variables on field k. That is, $I = \{\sum_{i=1}^{s} h_i g_i,\ h_i \in k[x_1, x_2, \cdots, x_d]\}$ for some $g_1, \cdots, g_s \in I$. Denoted by $I = \langle g_1, \cdots, g_s \rangle$.*

Proof: See Page 74, Cox, Little and O'Shea (1997).

By above theorem, since the complete aliasing structure of a design is contained in an ideal, it can be determined by a finite set of polynomials.

To find a basis of an ideal $I(V)$, it is essential to define a total ordering on the set of monomials

$$\{x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_d^{\alpha_d}, \alpha_i \geq 0\}.$$

A total ordering $\succ$ must have following properties:

(i) For any two non-identical momomials t_1 and t_2, $t_1 \succ t_2$ or $t_2 \succ t_1$;

(ii) $t_1 \succ t_2 \Rightarrow t_1 t_3 \succ t_2 t_3$ for any monomial t_3;

(iii) There is a minimal element of each non-empty subset.

There are finitely many monomial ordering. Among them, *lexicographic ordering* is the simplest and most basic one. Consider two monomial terms of d variables, $t_1 = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_d^{\alpha_d}$ and $t_2 = x_1^{\beta_1} x_2^{\beta_2} \cdots x_d^{\beta_d}$. Under lexicographic ordering, $t_1 \succ_{lex} t_2$, if and only if the left most nonzero coordinate of $(\alpha_1 - \beta_1, \alpha_2 - \beta_2, \cdots, \alpha_d - \beta_d)$ is positive. Another useful ordering is called *graded reverse lexicographic*. It compares total degrees of two monomials first, in which $t_1 \succ_{grevlex} t_2$, if and only if $\sum_i \alpha_i > \sum_i \beta_i$, or $\sum_i \alpha_i = \sum_i \beta_i$ and the right-most nonzero entry of $(\alpha_1 - \beta_1, \alpha_2 - \beta_2, \cdots, \alpha_d - \beta_d)$ is negative. In general, any total ordering of monomials of d variables can be defined by a $d \times d$ matrix $U = [u_1, u_2, \cdots, u_d]^T$ where u_i's are vectors with d elements. If $\alpha = (\alpha_1, \alpha_2, \cdots, \alpha_d)$ and $\beta = (\beta_1, \beta_2, \cdots, \beta_d)$, then $t_1 \succ t_2$ if and only if the leftmost nonzero coordinate of

$$((\alpha - \beta) \cdot u_1, (\alpha - \beta) \cdot u_2, \cdots, (\alpha - \beta) \cdot u_d)$$

is positive. Given a total monomial ordering, the leading monomial of a polynomial is well defined.

A Gröbner basis of $I(V)$ is basis which has the following property: the ideal generated by the leading monomials of the basis is the collection of the leading monomials of the polynomials in $I(V)$.

Definition 3 *Let I be an ideal in a polynomial ring of d variables, denote $LT(I)$ the set of leading terms of elements of I. For a fixed monomial ordering, a finite subset $G = \{g_1, g_2, \cdots, g_s\}$ of I is said to be a Gröbner basis if $\langle LT(g_1), \cdots, LT(g_s)\rangle = LT(I)$.*

Corollary 4 *A Gröbner basis is a basis of ideal I.*

The proof of the corollary is contained in the proof of the Hilbert basis theorem which can be found in Cox, *et. al.* (1997).

Given a fixed monomial ordering, the Gröbner basis is, however, not unique. Reduced Grönber basis of $I(V)$ is unique for a given total monomial ordering.

Definition 5 *A reduced Grn̈ber basis for a polynomial ideal I is a Gröbner basis G for I such that:*
(i) leading coefficient of g is 1 for all $g \in G$.
(ii) For all $g \in G$, no monomial of g lies in $\langle LT(G - \{g\}) \rangle$.

In the definition, $LT(G-\{g\})$ denote the leading terms of $G-\{g\}$, where $\langle LT(G-\{g\}) \rangle$ denotes the ideal generated by $LT(G-\{g\})$.

An efficient algorithm, Buchberger-Möller algorithm, have been developed to obtained the reduced Gröbner basis of $I(V)$ where V is a set of points in R^d. CoCoA, a computational algebraic geometry software package, is freely available over the internet. It allows users to specify any monomial ordering and has a build-in function **IdealOfPoints** which computes the reduced Gröbner bases of varieties. All the computation in this paper is done using CoCoA. General purpose symbolic mathematics software such as Maple and Mathematica also have a few build-in functions for computational algebraic geometry.

Pistone and Wynn (1996) study the 2^{6-2} factorial design as shown in Table 3. Using Maple, they obtain its Gröbner basis

Table 3: 2^{6-2} fractional factorial design

x_1	x_2	x_3	x_4	x_5	x_6
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

under lexicographic order:

$$\{x_6 - x_1x_2x_3,\ x_5 + x_2x_3,\ x_4 + x_1x_2,\ x_3^2 - 1,\ x_2^2 - 1,\ x_1^2 - 1\}.$$

One can easily observe that three polynomials in this Gröbner basis are the defining relations of the 2^{6-2} design:

$$x_4 = -x_1x_2,\ x_5 = -x_2x_3,\ x_6 = x_1x_2x_3.$$

Pistone and Wynn (1996) also compute the Gröbner basis of the 3^{4-2} fraction factorial design given in Table 1. They set the three levels $\{0, 1, 2\}$ to be $\{-1, 0, 1\}$. Its Gröbner basis is

$$\begin{aligned}\{\ & 4x_4 + 9x_1^2x_2^2 + 3x_1x_2^2 - 6x_2^2 - 3x_1^2x_2 + 3x_1x_2 + 2x_2 + 4 - 2x_1 - 6x_1^2,\\ & 4x_3 - 9x_1^2x_2^2 - 3x_1x_2^2 + 6x_2^2 - 3x1^2x_2 + 3x_1x_2 + 2x_2 - 4 + 6x_1^2 + 2x_1,\\ & x_2^3 - x_2,\ x_2^3 - x_2\ \}\end{aligned}$$

This, however, gives little inside information on the aliasing structure of the design.

Table 4: A Gröbner basis of 3^{4-2} factorial design

$$
\begin{aligned}
&A_q^2 + A_q - 2, \\
&A_l A_q - A_l, \\
&A_l^2 - 1/3A_q - 2/3, \\
&B_q^2 + B_q - 2, \\
&B_l B_q - B_l, \\
&B_l^2 - 1/3B_q - 2/3, \\
&C_q + 3/4B_l A_l + 3/4B_l A_q + 3/4B_q A_l - 1/4B_q A_q, \\
&C_l + 3/4B_l A_l - 1/4B_l A_q - 1/4B_q A_l - 1/4B_q A_q, \\
&D_q - 3/4B_l A_l + 3/4B_l A_q - 3/4B_q A_l - 1/4B_q A_q, \\
&D_l + 3/4B_l A_l + 1/4B_l A_q - 1/4B_q A_l + 1/4B_q A_q
\end{aligned}
$$

To reveal the aliasing structure of the design for linear-quadratic system, I compute a Gröbner basis of the contrast matrix (Table 2) of the 3^{4-2} design. Table 4 lists a Gröbner basis of the contrast matrix. The first three polynomials in the table describe the relation between the linear and the quadratic contrasts of factor A; the next three do the same for factor B. The last four polynomials resemble the defining relations which define the linear and quadratic contrasts of factor C and D in terms of the contrasts of factors A and B. For example, since $C_l + 3/4B_l A_l - 1/4B_l A_q - 1/4B_q A_l - 1/4B_q A_q$ is zero at all design points, the linear contrasts C_l is the linear combination of A_lB_l, A_lB_q, A_qB_l, and A_qB_q. In other words, the estimation of linear effect of C is confounded with all four components of AB interactions. In next section, I will show that such kind of Gröbner basis exist for a large group of factorial designs under a particular monomial ordering.

3 GENERALIZED DEFINING RELATION

For the 3^{4-2} fractional factorial design, its defining relations $C = AB$ and $D = AB^2$ have only combinatorial meaning and do not give us the aliasing relations between the contrasts of the linear-quadratic system. Moreover, for mixed-level designs such as OA(18,$2^1 3^7$), better known as L18 and OA(12,$2^4 3^1$), there is no defining relation in the combinatorial sense. In this section, I will introduce generalized defining relations which exist for a large group of factorial designs. I will also show that the generalized defining relations are part of a Gröbner basis of the contrast matrix of a design.

Theorem 6 *Consider a full factorial design $OA(n, s_1^1 s_2^1 \cdots s_m^1)$, where $n = \prod_{i=1}^n s_i$, s_i is the number of levels of factor X_i. Let $\{X_{i,c_1}, X_{i,c_2}, \cdots, X_{i,c_{s_i-1}}\}$ be $s_i - 1$ orthogonal contrasts of factor X_i and $X_{i,c_0} = \mathbf{1}$. The collection of vectors*

$$\{X_{1,c_{\alpha_1}} X_{2,c_{\alpha_2}} \cdots X_{m,c_{\alpha_m}}, 0 \le \alpha_i \le s_i - 1\} \tag{1}$$

is an orthogonal basis of R^n. In (1), all but $X_{1,c_0} X_{2,c_0} \cdots X_{m,c_0}$ are contrasts. $X_{1,c_0} X_{2,c_0} \cdots X_{m,c_0}$ is the constant term.

Proof: It is well know that for $i \neq j$, contrasts X_{i,t_1} and X_{j,t_2} are orthogonal. That is, the inner product of the two is zero. Since the strength of OA($n, s_1^1 s_2^1 \cdots s_m^1$) is m, it is easy to prove that

$$\sum_{i=1}^{n} X_{1,t_1}[i] X_{2,t_2}[i] \cdots X_{m,t_m}[i] = 0, \tag{2}$$

where $y[i]$ is the i^{th} elements of a vector y, X_{j,t_j}'s are not all $\mathbf{1}$'s. The left side of (2) can be seen as the generalized inner product of vectors $X_{1,t_1}, X_{2,t_2}, \cdots X_{m,t_m}$. Therefore, $X_{1,t_1}X_{2,t_2}\cdots X_{m,t_m}$ is a contrast. It can be easily seen that a monomial term of a single factor X, $X_{c_1}^{\gamma_1}X_{c_2}^{\gamma_2}\cdots X_{c_s-1}^{\gamma_s-1}$, is a linear combination of $X_{c_0}, X_{c_1}, \cdots, X_{c_s}$:

$$X_{c_1}^{\gamma_1}X_{c_2}^{\gamma_2}\cdots X_{c_s}^{\gamma_s} = a_0X_{c_0} + a_1X_{c_1} + \cdots + a_{s-1}X_{c_{s-1}}.$$

Moreover, if $\gamma_i \leq 1$ for all i, $a_0 = 0$ since $X_{c_1}^{\gamma_1}X_{c_2}^{\gamma_2}\cdots X_{c_s}^{\gamma_s}$ is orthogonal to X_{c_0}

Now, consider two contrasts,

$$C_1 = X_{1,c_{\alpha_1}}X_{2,c_{\alpha_2}}\cdots X_{m,c_{\alpha m}}$$

and

$$C_2 = X_{1,c_{\beta_1}}X_{2,c_{\beta_2}}\cdots X_{m,c_{\beta m}}.$$

To prove they are orthogonal, it is equivalent to prove that the generalized inner product of $X_{1,c_{\alpha_1}}, X_{1,c_{\beta_1}}, X_{2,c_{\alpha_2}}, X_{2,c_{\beta_2}}, \cdots, X_{m,c_{\alpha m}}, X_{2,c_{\beta m}}$ is zero. Since the monomial term $X_{i,c_{\alpha_i}}X_{i,c_{\beta_i}}$ involves only X_i, it can be written as a linear combination of $X_{i,c_1}, X_{i,c_2}, \cdots, X'_{i,c_{s_i}}s$. Consequently,

$$X_{1,c_{\alpha_1}}X_{1,c_{\beta_1}}X_{2,c_{\alpha_2}}X_{2,c_{\beta_2}}\cdots X_{m,c_{\alpha m}}X_{m,c_{\beta m}}$$

is a linear combination of $X_{1,t_1}X_{2,t_2}\cdots X'_{m,t_m}s$. Since $C_1 \neq C_2$, there is at least one i, such that $c_{\alpha_i} \neq c_{\beta_i}$. Therefore, $X_{1,c_0}X_{2,c_0}\cdots X_{m,c_0}$ must not be in the linear combination. By (2),

$$\sum_{i=1}^{n}(X_{1,c_{\alpha_1}}X_{1,c_{\beta_1}}X_{2,c_{\alpha_2}}X_{2,c_{\beta_2}}\cdots X_{m,c_{\alpha m}}X_{m,c_{\beta m}})[i] = 0 \qquad (3)$$

Thus, contrasts C_1 and C_2 are orthogonal. Consequently, the constant term, the main contrasts of the m factors and their interactions form an orthogonal basis of R^n. The proof is completed.

□

Corollary 7 *Let D be a design with m factors. Suppose the first l columns is an orthogonal array with strength l. The main contrasts of last $m-l$ factors are the linear combinations of the main contrasts of the first l factors and their interactions.*

Proof: The main contrasts of last $m - l$ factors are orthogonal to the constant term. By above theorem, they must be the linear combination of main contrasts of the first l factors and their interactions. □

Based on the Corollary above, for those designs whose projections on a subspace is a full factorial design, a set of generalized defining relations can be defined. The defining relations of regular two-level fractional factorial designs are its special cases.

Definition 8 *Let D be a design as in Corollary 7. Define $s_i - 1$ orthogonal contrasts for each factor X_i. The representations of a main contrasts C of the last $m-l$ factors as a linear combinations of the main and interaction contrasts of the first l factors is called the generalized defining relation of the contrast C. The collection of generalized defining relations of all main contrasts of the last $m - l$ factors is called the generalized defining relations of design D.*

The generalized defining relations defined above can be obtained using linear algebra. The coefficient of the defining relations can be determined by inner-products of the contrasts. The remaining question is, given generalized defining relations of a design, are they sufficient to determine all geometric aliasing relations of the design? The answer is positive and will be shown by Gröbner basis method.

Consider a contrast matrix V of a factorial design. The variables in the matrix are main contrasts of the factors. The ideal $I(V)$ contains all the geometric aliasing relations of our interest. The polynomials in $I(V)$ are in terms of main contrasts of each factor and their interactions. Each polynomial in the ideal associates with a geometric aliasing relation of the contrasts. I will show that under certain monomial orders, the generalized defining relations of a design are members of the Gröbner basis of the ideal. Moreover, a contrast defined by a defining relation does not appear in other members of the basis.

Let the contrasts in the matrix be in the order

$$\{X_{1,1}, X_{1,2}, \cdots, X_{1,s_1-1}, \cdots, X_{m,1}, X_{m,2}, \cdots, X_{1,s_1-1}\},$$

where $X_{i,j}$ is the j^{th} contrast of the factor X_i. A total monomial ordering is defined by

$$U = A \otimes B \tag{4}$$

where $\otimes$ is the Kronecker product, and

$$A = \begin{bmatrix} 1 & \cdots & 1 & 1 & 1 \\ 0 & \cdots & 0 & 0 & -1 \\ 0 & \cdots & 0 & -1 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & 0 \end{bmatrix}, B = \begin{bmatrix} 0 & \cdots & 0 & 1 \\ 0 & \cdots & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \cdots & 0 & 0 \end{bmatrix}.$$

Under this monomial ordering, the factors in the two monomial terms are compared first; if both have the same leading factor, the components of the leading factor are compared using the *graded reverse lexicographic* ordering. For example, the monomial ordering of main contrasts of 3^{4-2} factorial design is defined by

$$U = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

For example, under this ordering, $D_l \succ C_l \succ B_l \succ A_l$, $C_lD_l \succ B_lD_l$, $C_lC_qD_l \succ C_lD_l$.

The following theorem states that under the monomial ordering defined by (4), the reduced Gröbner basis of the contrast matrix contains the generalized defining relations.

Theorem 9 *Let D be a design as in Corollary 7 and V be its contrast matrix. Define the monomial ordering U as in (4). Let G_i be the reduced Gröbner basis of the contrast matrix of fac-*

tor X_i: $V_i = [X_{i,1}, X_{i,2}, \cdots, X_{i,s_i-1}]$ under graded reverse lexicographic ordering, for $i = 1, 2, \cdots, l$. Let $g_{ij} = X_{ij} - f_{ij}$, where f_{ij} is the generalized defining relation of X_{ij}, $i = l+1, \cdots, m$. Then

$$G = (\cup_{i=1}^{l} G_i) \cup (\cup_{i=l+1}^{m} \cup_{j=1}^{s_i-1} \{g_{ij}\})$$

is the reduced Gröbner basis of $I(V)$ under total monomial ordering U.

Proof: First, I will show that $LT(G_i) = \{X_{i,r}X_{i,t}, 1 \le r \le t \le s_i - 1\}$. Since $X_{i,1}, \cdots, X_{i,s_i-1}$ are linearly independent, a leading term of $I(V_i)$ must not be $X_{i,c}$. Therefore, for $g \in LT(I(V_i))$, it has to be divisible by one of the $X_{i,r}X_{i,t}$'s. Hence, $L(G_i) \supset \{X_{i,r}X_{i,t}, 1 \le r \le t \le s_i - 1\}$. Since $X_{i,r}X_{i,t}$'s are all linear combinations of $\mathbf{1}, X_{i,1}, X_{i,2}, \cdots, X_{i,s_i-1}$'s, $X_{i,r}X_{i,t} \in LT(I(V_i))$ for all $0 \le r \le t \le s_i - 1$. Hence, $LT(G_i) \subset \{X_{i,r}X_{i,t}, 1 \le r \le t \le s_i - 1\}$.

Now I will prove that $LT(I(V))$ is generated by $LT(G)$. First, consider a polynomial g in $I(V)$ whose leading term involves $X_{i,j}$ for $i > l$. $LT(g)$ is divisible by $LT(g_{ij}) = X_{i,j}$. Second, for a polynomial g in $I(V)$ whose leading term only involves first l factors, $LT(g)$ must not be in the form of $X_{1,t_1}X_{2,t_2}\cdots X_{l,t_l}$, since $\{X_{1,t_1}X_{2,t_2}\cdots X_{l,t_l}, t_i \in \{c_0, \cdots, c_{s_i-1}\}\}$ are linearly independent. Hence, $LT(g)$ is divisible by some elements in $\cup_{i=1}^{l} LT(G_i)$. Therefore, G is a Gröbner basis.

To prove that G is also a reduced Gröbner basis, it is sufficient to prove that no monomial of g_{ij} lies in $\langle LT(G - \{g_{ij}\})\rangle$. This can be easily seen since $X_{i,j}$ must not be in $\langle LT(G - \{g_{ij}\}) \rangle$ and $X_{1,t_1} X_{2,t_2} \cdots X_{l,t_l}$ must not either. The proof is now completed.

$\square$

From Theorem 9, the reduced Gröbner basis contains two kind of elements. One is the order-2 terms of contrasts of factor X_i as linear combination of main contrasts of X_i for $i \leq l$. The other is the defining relations of main contrasts of $X_i, i \geq l+1$ as linear combinations of main contrasts and interaction contrasts of factors $X_1, \cdots, X_l$. The two kinds of polynomials generate $I(V)$ which contains all geometric aliasing relations of a design.

The computational algebra geometry software package CoCoA allows users to specify a monomial ordering. Therefore, it can be used to obtain the generalized defining relations of a design by computing the reduced Gröbner basis of its contrast matrix. In the next section, we will study the aliasing structure of two commonly used designs.

4 TWO EXAMPLES

4.1 3^{3-1} Fractional Factorial Design

In Chapter 5, Wu and Hamada (2000) studies a 3^{3-1} fractional factorial design in which $C = AB$. This design is the first three columns of the design in Table 1 and its Gröbner basis consists of the first eight polynomials in Table 4. Besides the six main contrasts, two interaction terms are allowed to be added in the model. The defining relation of the design shows that both C_l

and C_q are linear combinations of all four components of AB interaction. Therefore, any pairs of the four components are not linearly dependent with six linear main effects. Consequently, any pair of AB interaction components can be added into the model.

Table 5 shows another 3^{3-1} fractional factorial design in which $C = A^2B^2 = -AB$. This design is considered isomorphic to the design $C = AB$ in the combinatorial sense. Using the Gröbner basis method, its defining relations are found and listed in Table 6. One can observe that C_l and C_q are linearly dependent with two AB interaction components each. Therefore, aliasing structure of two designs are different. This phenomenon has been found by S.W. Cheng in his unpublished Ph.D dissertation (1998) in which he studies 27 run three-level fractional factorial designs. He also referred this difference among combinatorial isomorphic designs as model non-isomorphic. Using the second design, A_lB_l and A_qB_q cannot be added into the model together, since the model would then be not estimable, neither do A_lB_q,A_qB_l. Other pairs, however, can be added into the model. However, the interaction components added are orthogonal with five main effect contrasts instead of only four in the first design.

4.2 L18 design

L18 which is shown in Table 7 is one of the most popular designs among industrial experimenters. Its aliasing structure is complicated and it has no defining relations in the combinatorial sense. However, since its first three columns is a full factorial

Table 5: 3^{3-1} fractional factorial design with $C = -AB$

A	B	C
0	0	0
0	1	2
0	2	1
1	0	2
1	1	1
1	2	0
2	0	1
2	1	0
2	2	2

Table 6: Defining relations of 3^{3-1} fractional factorial design with $C = -AB$

$$
\begin{aligned}
&A_q^2 + A_q - 2 = 0,\\
&A_l A_q - A_l = 0,\\
&A_l^2 - 1/3A_q - 2/3 = 0,\\
&B_q^2 + B_q - 2 = 0,\\
&B_l B_q - B_l = 0,\\
&B_l^2 - 1/3B_q - 2/3 = 0,\\
&C_q - 3/2A_l B_l + 1/2A_q B_q = 0,\\
&C_l - 1/2A_l B_q - 1/2A_q B_l = 0
\end{aligned}
$$

design, its generalized defining relations can be obtained using the method described in the previous section. Table 8 shows a Gröbner basis of L18 containing its defining relations. From the table, one can observe that how main contrasts of y_3 to y_7 are linear combinations of contrasts of x, y_1 and y_2. It can be seen that interactions between x and y_1 are not in the defining relations of factors y_3 to y_7, this means that x and y_1 interaction is not aliased with any of the main contrasts. This provides an important piece of information for data analysis methods such as half-normal plot and Lenth method. This result has been known previously. However, our method reveals it in a simpler and more elegant fashion.

5 SUMMARY AND FUTURE RESEARCH

The aliasing structure is an important characteristic of a factorial design. In practice, it is a vital piece of information in selecting an efficient design for an experiment. Unfortunately, previous method only works well for regular two-level fractional factorial designs. This paper establishes a new framework for studying aliasing structures of multi-level and mixed-level designs. The new framework is build on *geometric aliasing*. The aliasing relations of the two-level factorial designs are special cases of geometric aliasing. Geometric aliasing extends the aliasing relation in two-level factorial design naturally to all experimental designs. It also has a nice geometric interpretation. In the new framework,

Table 7: The L18 orthogonal array

x	y_1	y_2	y_3	y_4	y_5	y_6	y_7
1	1	1	1	1	1	1	1
1	1	2	2	2	2	2	2
1	1	3	3	3	3	3	3
1	2	1	1	2	2	3	3
1	2	2	2	3	3	1	1
1	2	3	3	1	1	2	2
1	3	1	2	1	3	2	3
1	3	2	3	2	1	3	1
1	3	2	1	3	2	1	2
2	1	1	3	3	2	2	1
2	1	2	1	1	3	3	2
2	1	3	2	2	1	1	3
2	2	2	3	1	2	1	3
2	2	3	1	2	3	2	1
2	3	1	3	2	3	1	2
2	3	2	1	3	1	2	3
2	3	3	2	1	2	3	1

Table 8: Gröbner basis of the contrast matrix of L18. y_{i1} and y_{i2} are the linear and quadratic contrasts of factor y_i respectively.

$$
\begin{array}{l}
x^2 - 1, \\
y_{12}^2 - y_{12} - 2, \\
y_{11}y_{12} + y_{11}, \\
y_{11}^2 + 1/3y_{12} - 2/3, \\
y_{22}^2 - y_{22} - 2, \\
y_{21}y_{22} + y_{21}, \\
y_{21}^2 + 1/3y_{22} - 2/3, \\
y_{32} - 3/8xy_{11}y_{21} + 3/8y_{11}y_{21} + 5/8xy_{12}y_{21} + 3/8y_{12}y_{21} - 1/2xy_{21} \\
-3/8xy_{11}y_{22} + 3/8y_{11}y_{22} + 1/8xy_{12}y_{22} - 1/8y_{12}y_{22} + 1/2xy_{22}, \\
y_{31} - 3/8xy_{11}y_{21} + 3/8y_{11}y_{21} + 1/8xy_{12}y_{21} - 1/8y_{12}y_{21} + 1/2xy_{21} \\
+1/8xy_{11}y_{22} - 1/8y_{11}y_{22} - 5/24xy_{12}y_{22} - 1/8y_{12}y_{22} + 1/6xy_{22}, \\
y_{42} + 3/4xy_{11}y_{21} + 3/4y_{11}y_{21} - 1/2xy_{12}y_{21} - 1/2xy_{21} - 1/4xy_{12}y_{22} \\
+1/4y_{12}y_{22} + 1/2xy_{22}, \\
y_{41} - 1/4xy_{12}y_{21} + 1/4y_{12}y_{21} + 1/2xy_{21} - 1/4xy_{11}y_{22} - 1/4y_{11}y_{22} \\
+1/6xy_{12}y_{22} + 1/6xy_{22}, \\
y_{52} - 3/8xy_{11}y_{21} - 9/8y_{11}y_{21} - 3/8xy_{12}y_{21} + 3/8y_{12}y_{21} - 3/8xy_{11}y_{22} \\
+3/8y_{11}y_{22} - 3/8xy_{12}y_{22} - 1/8y_{12}y_{22}, \\
y_{51} - 3/8xy_{11}y_{21} + 3/8y_{11}y_{21} - 3/8xy_{12}y_{21} - 1/8y_{12}y_{21} + 1/8xy_{11}y_{22} \\
+3/8y_{11}y_{22} + 1/8xy_{12}y_{22} - 1/8y_{12}y_{22}, \\
y_{62} - 3/4xy_{11}y_{21} - 3/4y_{12}y_{21} - 3/4xy_{11}y_{22} + 1/4y_{12}y_{22}, \\
y_{61} - 3/4xy_{11}y_{21} + 1/4y_{12}y_{21} + 1/4xy_{11}y_{22} + 1/4y_{12}y_{22}, \\
y_{72} + 3/4xy_{11}y_{21} + 1/4xy_{12}y_{21} + xy_{21} + 3/4y_{11}y_{22} + 1/4y_{12}y_{22}, \\
y_{71} + 3/4y_{11}y_{21} + 1/4y_{12}y_{21} - 1/4xy_{11}y_{22} - 1/12xy_{12}y_{22} - 1/3xy_{22}
\end{array}
$$

geometric aliasing can be studied using theories and algorithms in computational algebraic geometry. The future study will focus on the generalization of design efficiency criteria such as resolution and aberration under the new framework, and the aliasing structures of useful multi-level and mixed-level factorial designs.

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