Characterizations of indicator functions of fractional factorial designs

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Abstract

A polynomial indicator function of designs is first introduced by Fontana, Pistone and Rogantin (2000) for two-level designs. They give the structure of the indicator function of two-level designs, especially from the viewpoints of the orthogonality of the designs. Based on the structure, they use the indicator functions to classify all the orthogonal fractional factorial designs with given sizes using computational algebraic software. In this paper, generalizing the results on two-level designs, the structure of the indicator functions for multi-level designs is derived. We give a system of algebraic equations for the coefficients of indicator functions of fractional factorial designs with given orthogonality. We also give another representation of the indicator function, a contrast representation, which reflects the size and the orthogonality of the corresponding design directly. We use these results to classify orthogonal $2^3 \times 3$ designs with strength 2 and orthogonal $2^4 \times 3$ designs with strength 3 by a computational algebraic software.

Keywords: Computational algebraic statistics, Fractional factorial designs, Gröbner bases, Indicator functions, Orthogonal designs.

1 Introduction

Applications of Gröbner basis theory to various problems of statistics arises in early 1990s. One of the first works in this developing field, a computational algebraic statistics, is given by Pistone and Wynn ([10]), where the Gröbner basis theory is applied to the identifiability problem in the design of experiments. After this work, various algebraic approaches to the problems in the design of experiments are presented by researchers both in the fields of algebra and statistics. A theory of the indicator function of fractional factorial designs is one of the early results in this branch.

The indicator function is first introduced by Fontana, Pistone and Rogantin ([5]) for two-level fractional factorial designs. In [5], based on the results of [10], one-to-one correspondence between the design and its indicator function is shown. This correspondence enables us to translate various statistical concepts to algebraic concepts, i.e., various results on the fractional factorial designs can be interpreted to the structure of their indicator functions. For example, abberation and resolution are important concepts in design
of experiments, and there is a well-established history starting with [2] for two-level fractional factorial designs. An important contribution of [5] is to characterize these concepts as the structure of the indicator functions.

To illustrate the motivation of this paper, we glance at the arguments of [5] by examples. Note that the necessary definitions on the designs and indicator functions will be given in Section 2. Figure 1 is examples of two-level fractional factorial designs. We code the levels of each factor as \{-1, 1\} according to [5]. For each design, each row of the table shows the combination of the levels of the factors \(x_i\)'s for each experimental run, and each column corresponds to each factor. For example, the design \(F_1\) is a fractional factorial design for 5 two-level factors \(x_1, \ldots, x_5\), composed of 8 points in \((-1, 1)^5\),

\[
\{(1, 1, 1, 1, 1), (1, 1, -1, 1, -1), \ldots, (-1, -1, -1, 1, 1)\}.
\]

In the field of design of experiments, \(F_1\) is known as a regular fractional factorial design with the defining relation \(x_1x_2x_4 = x_1x_3x_5 = 1\). On the other hand, the design \(F_2\) is an example of nonregular designs. For details on the regularity of designs, see [11] for example.

The indicator functions of \(F_1\) and \(F_2\) are given as follows, respectively.

\[
\begin{align*}
F_1 : & \quad f_1(x_1, x_2, x_3, x_4, x_5) = \frac{1}{4} + \frac{1}{4}(x_1x_2x_4 + x_1x_3x_5 + x_2x_3x_4x_5) \\
F_2 : & \quad f_2(x_1, x_2, x_3, x_4) = \frac{3}{8} - \frac{1}{8}x_4 + \frac{1}{8}(x_1x_2 + x_1x_3 - x_2x_3) + \frac{1}{8}(x_1x_3x_4 + x_2x_3x_4) + \frac{3}{8}x_2x_3x_4
\end{align*}
\]

We see, for example, \(f_1(x_1, \ldots, x_5) = 1\) for 8 points in \(F_1\), and \(f_1(x_1, \ldots, x_5) = 0\) for the other 24 points not in \(F_1\). The indicator function of the design of \(n\) two-level factors, \(x_1, x_2, \ldots, x_n\) has a unique polynomial representation of the form

\[
f(x_1, \ldots, x_n) = \sum_{a \in \{0, 1\}^n} \theta_a x^a, \tag{1}
\]
where \( \mathbf{x}^a = \prod_{i=1}^{n} x_i^{a_i} \) and \( a = (a_1, \ldots, a_n) \in \{0, 1\}^n \). As is shown in [5], the set of the coefficients \( \{\theta_a\}_{a \in \{0, 1\}^n} \) has all the information of the corresponding design. For example, we see the following facts from the coefficients of the indicator functions \( f_1 \) and \( f_2 \) for \( F_1 \) and \( F_2 \).

- The constant term \( \theta_{(0,\ldots,0)} \) shows the ratio between the size of the design to the size of the full factorial design. In fact, \( F_1 \) is a \( 1/4 \) fraction of the full factorial \( 2^5 \) design, and \( F_2 \) is a \( 3/8 \) fraction of the full factorial \( 2^4 \) design.

- The coefficient of the main effect term \( \theta_a, \sum_j a_j = 1 \) shows the “balance” of two levels for this factor. In fact, for \( F_1, \theta_{(1,0,0,0,0)} = \cdots = \theta_{(0,0,0,0,1)} = 0 \) shows \( F_1 \) is an equireplicated design, i.e., two levels appear equally often for each factor. On the other hand, for \( F_2, \theta_{(1,0,0,0,0)} = \theta_{(0,1,0,0,0)} = \theta_{(0,0,1,0,0)} = 0 \) and \( \theta_{(0,0,0,1,0)} \neq 0 \) show \( F_2 \) is equireplicated for factors \( x_1, x_2, x_3 \) but not for \( x_4 \).

- The coefficient of the two-factor interaction term \( \theta_a, \sum_j a_j = 2 \) shows the “orthogonality” of the design. In fact, for \( F_1, \theta_{(1,1,0,0,0)} = \cdots = \theta_{(0,0,0,1,1)} = 0 \) shows \( F_1 \) is an orthogonal design, i.e., possible combinations of levels, \((-1, -1), (-1, 1), (1, -1), (1, 1)\), appear equally often for each pair of the factors. On the other hand, for \( F_2, \theta_{(1,0,0,1,0)} = \theta_{(0,1,0,1,0)} = \theta_{(0,0,1,1,1)} = 0 \) shows that the factor \( x_4 \) is orthogonal to each of the other factors, whereas \( \theta_{(1,1,0,0)}, \theta_{(1,0,1,0)}, \theta_{(0,1,1,0)} \neq 0 \) shows that \( x_1, x_2, x_3 \) are not orthogonal in each other.

In other words, statistical concepts such as aberration and resolution can be related to the structure of the corresponding indicator functions directly for two-level designs. In particular, the structure of the indicator function of regular two-level designs can be characterized by their defining relations, and are fully revealed. See [12] for detail.

Another characterization of the indicator function of two-level designs relating the \( D \)-optimality of the design is given by the author in [1].

In [5], these structures of the indicator function are applied to the classification of the design, which is also the object of this paper. The argument of [5] is as follows. For the indicator function [1] of two-level designs, the set of the coefficients \( \{\theta_a\}_{a \in \{0, 1\}^n} \) satisfies a system of algebraic equations

\[
\theta_a = \sum_{a' \in \{0, 1\}^n} \theta_{a'} \theta_{a + a'}, \quad a \in \{0, 1\}^n,
\]

where the sum \( a + a' \) is considered under “mod 2” (Proposition 3.7 of [5]). Therefore, adding constraints for some orthogonality of the designs to [2], we have a system of algebraic equations having the designs with these orthogonality as the solutions. For example, for the case of \( n = 5 \), additional constraints

\[
\theta_{(0,0,0,0,0)} = \frac{1}{4}, \quad \theta_a = 0 \text{ for } \sum_j a_j = 1, 2
\]

(3)

to (2) yields a system of algebraic equations having all the orthogonal designs with the size 8 as the solution (and \( F_1 \) corresponds to one of the solutions). In this way, the complete
lists of the orthogonal designs for \( n = 4, 5 \) are computed by a computational algebraic software in [3]. Recall that solving a system of algebraic equations is a fundamental problem where the theory of Gröbner basis is used.

In this paper, we consider generalization of the above argument on two-level designs to general fractional factorial designs. Note that the direct relations between the size and orthogonality of designs and their indicator functions are obtained only for two-level designs. To see this, consider a fractional factorial design of three-level factors \( F_3 \) displayed in Figure 2. \( F_3 \) is a regular fractional factorial design with the defining relation

\[
\begin{align*}
  x_1 + x_2 + x_3 &= x_1 + 2x_2 + x_4 = 0 \pmod{3}.
\end{align*}
\]

Figure 2: A regular fractional factorial design for three-level factors with the defining relation \( x_1 + x_2 + x_3 = x_1 + 2x_2 + x_4 = 0 \pmod{3} \).

the resolution of \( F_3 \) is seen in its defining relation), the structure of its indicator function seems complicated as follows.

\[
f(x_1, x_2, x_3, x_4) = 1 - x_1^2 - x_2^2 - x_3^2 - x_4^2 + x_1^2 x_2^2 + x_1^2 x_3^2 + x_1^2 x_4^2 + x_2^2 x_3^2 + x_2^2 x_4^2 + x_3^2 x_4^2 \\
+ \frac{1}{4}(x_1^2 x_2 x_3 - x_1^2 x_2 x_4 + x_1^2 x_3 x_4 + x_1 x_2^2 x_3 + x_1 x_2^2 x_4 - x_2^2 x_3 x_4) \\
+ \frac{3}{4}(x_1^2 x_2^2 x_3^2 + x_1^2 x_2^2 x_4^2 + x_1^2 x_3^2 x_4^2 + x_2^2 x_3^2 x_4^2) \quad (4)
\]

There are several approaches to consider the indicator functions of multilevel designs. In [9], a complex coding is proposed to generalize the arguments on two-level cases to multilevel cases. For example, instead of \( \{-1, 0, 1\} \) above, the three-level factor is coded as \( \{1, w, w^2\} \), where \( w = \exp(2\pi \sqrt{-1}/3) \) in [9]. Another approach is presented in [3] for the real coefficients field. However, it is better if we can consider \( \mathbb{Q} \), the field of rational numbers, as the coefficients field, because algebraic computations are conducted in \( \mathbb{Q} \) (or finite fields \( \mathbb{Z}/p\mathbb{Z} \)) for standard computational algebraic software. In this paper, we give generalization of the relations for two-level designs such as (2) and (3) to general multilevel designs for the rational coefficients field \( \mathbb{Q} \), and show how to relate the structure of the designs to the structure of their indicator functions.
The construction of this paper is as follows. In Section 2, we give necessary definitions and theorems on the indicator functions. In Section 3, we give the structure of the indicator functions for general fractional factorial designs. We also derive another representation of the indicator functions, namely, contrast representation, to reflect the orthogonality of the designs directly. In Section 4, we use these results to classify $2^3 \times 3$ and $2^4 \times 3$ designs with given orthogonalities by a computational algebraic software.

2 The indicator functions of fractional factorial designs

In this section, we give necessary materials on the indicator functions of fractional factorial designs. The arguments are based on the theory of interpolatory polynomial functions on designs, which is one of the first applications of Gröbner basis theory to statistics introduced by [10]. See [8] or Chapter 5 of [4] for detail.

Let $x_1, \ldots, x_n$ be $n$ factors. Let $A_j \subset \mathbb{Q}$ be a level set of a factor $x_j$ for $j = 1, \ldots, n$, where $\mathbb{Q}$ denotes the field of rational numbers. We denote by $r_j = \#A_j$ the cardinality of $A_j$ and assume $r_j \geq 2$ for $j = 1, \ldots, n$. A full factorial design of the factors $x_1, \ldots, x_n$ is $D = A_1 \times \cdots \times A_n$. For later use, we introduce an index set

$$\mathcal{I} = \{(i_1, \ldots, i_n) \in [r_1] \times \cdots \times [r_n]\},$$

where $[k] = \{1, 2, \ldots, k\}$ for a positive integer $k$. We specify each point of $D$ as $D = \{d_i \in \mathbb{Q}^n : i \in \mathcal{I}\}$. When we code $A_j = [r_j]$ for $j = 1, \ldots, n$, $\mathcal{I}$ coincides with $D$ itself.

A subset of $D$ is called a fractional factorial design. A fractional factorial design $F \subset D$ can be written as $F = \{d_i \in D : i \in \mathcal{I}'\}$ where $\mathcal{I}'$ is a subset of $\mathcal{I}$. Each design can be viewed as a finite subset of $\mathbb{Q}^n$, i.e., as an algebraic variety. Therefore each design can be characterized as the set of the solutions of a system of polynomial equations with rational coefficients. The size of a design is the cardinality of the design. We write the size of a full factorial design $D$ as $m = \prod_{j=1}^n r_j$ for later use.

Let $\mathbb{Q}[x_1, \ldots, x_n]$ be the polynomial ring with coefficients in $\mathbb{Q}$. For a design $F \subset \mathbb{Q}^n$, we denote by $I(F)$ the set of polynomials in $\mathbb{Q}[x_1, \ldots, x_n]$ which are 0 at every point of $F$, i.e.,

$$I(F) = \{f \in \mathbb{Q}[x_1, \ldots, x_n] : f(d) = 0, \forall d \in F\}.$$

It is easy to prove that the set $I(F)$ is an ideal of $\mathbb{Q}[x_1, \ldots, x_n]$. $I(F)$ is called a design ideal of $F$. The design ideal introduced by [10] is a fundamental tool to consider designs algebraically. The design ideal is a radical ideal (Theorem 20 of [8]). The set of points $d \in \mathbb{Q}^n$ satisfying $f(d) = 0$ for all $f \in I(F)$ is $F$ itself.

For a full factorial design $D$, the design ideal $I(D)$ can be written as

$$I(D) = \langle x_j^{r_j} - g_j, \ j = 1, \ldots, n \rangle,$$

where $g_j$ is a polynomial in $\mathbb{Q}[x_j]$ with the degree less than $r_j$, $j = 1, \ldots, n$. In other words, the set

$$G = \{x_j^{r_j} - g_j, \ j = 1, \ldots, n\}$$
is a generator of $I(D)$. In addition, $G$ is a reduced Gröber basis of $I(D)$ for any monomial order. We write the set of the monomials that are not divisible by the initial monomials of $G$, \( \{x_j^{r_j}, \ j = 1, \ldots, n\} \), as

$$
\text{Est}(D) = \left\{ x^a = \prod_{j=1}^n x_j^{a_j} : \ a \in L \right\},
$$

where

$$
L = \{ a = (a_1, \ldots, a_n) \in \mathbb{Z}_{\geq 0}^n : 0 \leq a_j \leq r_j - 1, \ j = 1, \ldots, n \}
$$

and $\mathbb{Z}_{\geq 0}$ is the set of nonnegative integers. Note that the cardinality of $L$ is $m$. From $D = \{d_i \in \mathbb{Q}^n : i \in I\}$ and $L$, we define a model matrix by

$$
X = [d_i^a]_{i \in I, a \in L},
$$

where $d_i^a = \prod_{j=1}^n d_{ij}^{a_j}$ and $d_{ij}$ is the level of the factor $j$ in the experimental run indexed by $i \in I$. Note that $X$ is called a design matrix in Definition 26 of $[8]$. By ordering the elements of $I$ and $L$, $X$ is an $m \times m$ matrix, and is nonsingular (Theorem 26 of $[8]$).

The quotient of $\mathbb{Q}[x_1, \ldots, x_n]$ modulo the design ideal $I(D) \subset \mathbb{Q}[x_1, \ldots, x_n]$ is defined by

$$
\mathbb{Q}[x_1, \ldots, x_n]/I(D) = \{[f] : f \in \mathbb{Q}[x_1, \ldots, x_n]\},
$$

where we define $[f] = \{g \in \mathbb{Q}[x_1, \ldots, x_n] \text{ such that } f - g \in I(D)\}$. In the terminology of the designs of experiments, two polynomial models $f$ and $g$ are confounded on $D$ if and only if $f - g \in I(D)$. Therefore each element $[f] \in \mathbb{Q}[x_1, \ldots, x_n]/I(D)$ is the set of the polynomials $g \in \mathbb{Q}[x_1, \ldots, x_n]$ that is confounded to $f$ on $D$. An important fact is that $\text{Est}(D)$ is a basis of $\mathbb{Q}[x_1, \ldots, x_n]/I(D)$ as a $\mathbb{Q}$-vector space. See Theorem 15 of $[8]$ for detail.

Suppose we have a $\mathbb{Q}$-valued response (or, observations) $y = (y_i)_{i \in I}$ on $D = \{d_i \in \mathbb{Q}^n : i \in I\}$. Note that each polynomial $f \in \mathbb{Q}[x_1, \ldots, x_n]$ can be viewed as a response function on $D$, i.e., $f \in \mathbb{Q}^D$ where we denote $\mathbb{Q}^D$ by the vector space of functions from $D$ to $\mathbb{Q}$. The interpolatory polynomial function for $y$ is a polynomial $f \in \mathbb{Q}[x_1, \ldots, x_n]$ satisfying $f(d_i) = y_i$, $i \in I$. From the fact that $\text{Est}(D)$ is a basis of $\mathbb{Q}[x_1, \ldots, x_n]/I(D)$, the interpolatory polynomial function for $y$ is written uniquely as

$$
f(x_1, \ldots, x_n) = \sum_{a \in L} \theta_a x^a, \tag{5}
$$

where an $m \times 1$ column vector $\theta = (\theta_a)_{a \in L}$ is given by $\theta = X^{-1}y$ for an $m \times 1$ column vector $y$. See Theorem 26 of $[8]$ for detail.

Now we introduce an indicator function.

**Definition 2.1** ($[8]$). Let $F \subset D$ be a fractional factorial design. The indicator function of $F$ is a response function $f$ on $D$ satisfying

$$
f(d) = \begin{cases} 
1, & \text{if } d \in F, \\
0, & \text{if } d \in D \setminus F.
\end{cases}
$$
By the definition, the indicator function is constructed as follows. Write a fractional factorial design \( F \subseteq D \) as \( F = \{ d_i \in D : i \in I' \} \) for a subset \( I' \subseteq I \). Then the indicator function of \( F \) is the interpolatory polynomial function for a response \( y = (y_i)_{i \in I} \), where
\[
y_i = \begin{cases} 
1, & \text{if } i \in I' \\
0, & \text{if } i \in I \setminus I'.
\end{cases}
\]
(6)
From the uniqueness of the interpolatory polynomial function mentioned above, the representation of the indicator function is unique.

**Example 2.2.** Consider designs of 3 factors \( x_1, x_2, x_3 \), where \( x_1, x_2 \) are two-level factors and \( x_3 \) is a three-level factor. We code the levels of each factor as
\[
A_1 = A_2 = \{-1, 1\}, \quad A_3 = \{-1, 0, 1\}.
\]
Therefore \( r_1 = r_2 = 2, r_3 = 3 \), and the full factorial design \( D = A_1 \times A_2 \times A_3 \) has \( m = 12 \) points. The index set is \( I = \{1, 2\} \times \{1, 2\} \times \{1, 2, 3\} \). The full factorial design \( D \) is written as \( D = \{ d_i : i \in I \} \), where
\[
\begin{align*}
&d_{(1,1,1)} = (-1, -1, -1), \quad d_{(1,1,2)} = (-1, -1, 0), \quad d_{(1,1,3)} = (-1, -1, 1), \\
&d_{(1,2,1)} = (-1, 1, -1), \quad d_{(1,2,2)} = (-1, 1, 0), \quad d_{(1,2,3)} = (-1, 1, 1), \\
&d_{(2,1,1)} = (1, -1, -1), \quad d_{(2,1,2)} = (1, -1, 0), \quad d_{(2,1,3)} = (1, -1, 1), \\
&d_{(2,2,1)} = (1, 1, -1), \quad d_{(2,2,2)} = (1, 1, 0), \quad d_{(2,2,3)} = (1, 1, 1).
\end{align*}
\]
The design ideal of \( D \) is written as
\[
I(D) = \langle x_1^2 - 1, x_2^2 - 1, x_3^3 - 3 \rangle \subset \mathbb{Q}[x_1, x_2, x_3],
\]
and \( G = \{x_1^2 - 1, x_2^2 - 1, x_3^3 - 3\} \) is a reduced Gröbner basis of \( I(D) \) for any monomial order. Therefore we have
\[
\text{Est}(D) = \{1, x_1, x_2, x_3, x_1^2, x_2^2, x_1 x_2, x_1 x_3, x_2 x_3, x_1 x_2 x_3, x_1 x_2^2 x_3, x_2 x_3^2, x_1 x_2 x_3^2\}.
\]
Note that there are \( m \) monomials in \( \text{Est}(D) \). Corresponding \( L \) is given by
\[
L = \{(0, 0, 0), (1, 0, 0), (0, 1, 0), (0, 0, 1), (0, 0, 2), (1, 1, 0), (1, 0, 1), (0, 1, 1), (1, 1, 1), (1, 0, 2), (0, 1, 2), (1, 1, 2)\}.
\]
The model matrix \( X \) is given in Figure 3. Here, and hereafter, we write each element of \( L \) and \( I \) by omitting commas as \((a_1 \cdots a_n)\) or \((i_1 \cdots i_n)\) instead of \((a_1, \cdots, a_n)\) or \((i_1, \cdots, i_n)\) for simplicity.

Now consider a fractional factorial design \( F = \{ d_i : i \in I' \} \subseteq D \), where \( I' = \{(111), (122), (213), (223)\} \). The indicator function of \( F \) is constructed as the interpolatory polynomial function \((\ref{eq:indicator})\) for a response \( y = (y_i)_{i \in I} \) satisfying \((\ref{eq:unique})\). For this \( I' \), \( y = (1, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 1)^T \) and we have
\[
\theta = X^{-1}y = \frac{1}{8}(2, -2, 2, 1, 1, -2, 3, 1, -1, 3, -3, 3)^T,
\]
where \( ^T \) is a transpose. Therefore the indicator function of \( F \) is
\[
f(x_1, x_2, x_3) = \frac{1}{4} - \frac{1}{4}(x_1 - x_2) + \frac{1}{8}(x_3 + x_3) - \frac{1}{4}x_1 x_2 + \frac{3}{8}x_1 x_3 + \frac{1}{8}x_2 x_3
\]
\[- \frac{1}{8}x_1 x_2 x_3 + \frac{3}{8}(x_1 x_3^2 - x_2 x_3^2 + x_1 x_2 x_3^2).
\]
| $T \setminus L$ | 000  | 010  | 001  | 002  | 110  | 101  | 011  | 111  | 102  | 012  | 112  |
|--------------|------|------|------|------|------|------|------|------|------|------|------|
| 111          | 1    | −1   | −1   | −1   | 1    | 1    | 1    | −1   | −1   | −1   | 1    |
| 112          | 1    | −1   | −1   | 0    | 0    | 1    | 0    | 0    | 0    | 0    | 0    |
| 113          | 1    | −1   | −1   | 1    | 1    | 1    | −1   | −1   | 1    | −1   | −1   |
| 121          | 1    | −1   | 1    | −1   | 1    | 1    | −1   | 1    | −1   | 1    | −1   |
| 122          | 1    | −1   | 1    | 0    | 0    | 0    | −1   | 0    | 0    | 0    | 0    |
| 123          | 1    | −1   | 1    | 1    | 1    | −1   | 1    | −1   | 1    | −1   | 1    |
| 211          | 1    | 1    | −1   | −1   | 1    | −1   | −1   | 1    | 1    | −1   | −1   |
| 212          | 1    | 1    | −1   | 0    | 0    | −1   | 0    | 0    | 0    | 0    | 0    |
| 213          | 1    | 1    | −1   | 1    | 1    | −1   | 1    | −1   | 1    | −1   | −1   |
| 221          | 1    | 1    | 1    | −1   | 1    | 1    | −1   | −1   | 1    | 1    | 1    |
| 222          | 1    | 1    | 1    | 0    | 0    | 1    | 0    | 0    | 0    | 0    | 0    |
| 223          | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |

Figure 3: The model matrix of a full factorial design $D = \{-1, 1\}^2 \times \{-1, 0, 1\}$.

### 3 Characterization of orthogonal fractional factorial designs by indicator functions

Now we consider relations between the design and its indicator function. We start with the generalization of the relation (2) for two-level designs to multilevel designs.

A polynomial $f \in \mathbb{Q}[x_1, \ldots, x_n]$ is an indicator function of some fractional factorial design $F \subset D = \{d_i \in \mathbb{Q}^n : i \in T\}$ if and only if $f^2 - f \in I(D)$, i.e., $f$ and $f^2$ are in the same equivalence class of $\mathbb{Q}[x_1, \ldots, x_n]/I(D)$. Therefore, suppose $f$ represented as (5) is an indicator function of some fractional factorial design, we have

$$
\sum_{a \in L} \theta_a x^a = \left(\sum_{a \in L} \theta_a x^a\right)^2 \mod I(D) = \sum_{a_1 \in L} \sum_{a_2 \in L} \theta_{a_1} \theta_{a_2} x^{a_1 + a_2} \mod I(D).
$$

Here, write the standard form of $\sum_{a_1 \in L} \sum_{a_2 \in L} \theta_{a_1} \theta_{a_2} x^{a_1 + a_2}$ with respect to $G$ as

$$
r = \sum_{a \in L} \mu_a x^a.
$$

In other words, $r$ is a unique remainder when we divide $\sum_{a_1 \in L} \sum_{a_2 \in L} \theta_{a_1} \theta_{a_2} x^{a_1 + a_2}$ by $G$, the reduced Gröber basis of $I(D)$. Then we have the following result.

**Proposition 3.1** (Generalization of Proposition 3.7 of [5]). A polynomial $f$ represented as (5) is an indicator function of some fractional factorial design if and only if a system of algebraic equations

$$
\theta_a = \mu_a, \quad a \in L
$$

holds, where $\mu_a$ is given by (7).
Proof. From the division algorithm and the property of the Gröbner basis. See Chapter 2 of [4].

Example 3.2 (Continuation of Example 2.2). Consider $2 \times 2 \times 3$ designs. When we code the levels as $A_1 = A_2 = \{-1, 1\}, A_3 = \{-1, 0, 1\}$, the relation (8) is as follows.

\[
\begin{align*}
\theta_{000} &= \theta_0^2 + \theta_1^2 + \theta_2^2 + \theta_3^2 \\
\theta_{100} &= 2\theta_0\theta_1^2 + \theta_1^2 + \theta_2^2 + \theta_3^2 \\
\theta_{010} &= 2\theta_1^2 + \theta_0\theta_2^2 + \theta_1^2 + \theta_3^2 \\
\theta_{001} &= 2\theta_0\theta_1 + 2\theta_0\theta_2 + 2\theta_0\theta_3 + 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{002} &= 2\theta_0\theta_1 + 2\theta_0\theta_2 + 2\theta_0\theta_3 + 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{110} &= 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{111} &= 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{112} &= 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{12} &= 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{13} &= 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{2} &= 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{3} &= 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\end{align*}
\]

Each solution of the above system of polynomial equations corresponds to the coefficients of the indicator function for each fractional factorial designs.

If we change the level codings, the relation (8) changes. For example, when we code the levels as $A_1 = A_2 = \{0, 1\}, A_3 = \{0, 1, 2\}$, the relation (8) is as follows.

\[
\begin{align*}
\theta_{000} &= \theta_0^2 \\
\theta_{100} &= \theta_0^2 + 2\theta_0\theta_1 \\
\theta_{010} &= \theta_0^2 + 2\theta_0\theta_2 \\
\theta_{001} &= -4\theta_0\theta_2 + 6\theta_0^2 + 2\theta_0\theta_1 \\
\theta_{002} &= \theta_0^2 + 6\theta_0\theta_2 + 2\theta_0\theta_1 \\
\theta_{110} &= 2\theta_0\theta_1 + 2\theta_0\theta_2 + 2\theta_0\theta_3 + 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{111} &= 2\theta_0\theta_1 + 2\theta_0\theta_2 + 2\theta_0\theta_3 + 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{112} &= 2\theta_0\theta_1 + 2\theta_0\theta_2 + 2\theta_0\theta_3 + 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{12} &= 2\theta_0\theta_1 + 2\theta_0\theta_2 + 2\theta_0\theta_3 + 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{13} &= 2\theta_0\theta_1 + 2\theta_0\theta_2 + 2\theta_0\theta_3 + 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{2} &= 2\theta_0\theta_1 + 2\theta_0\theta_2 + 2\theta_0\theta_3 + 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\theta_{3} &= 2\theta_0\theta_1 + 2\theta_0\theta_2 + 2\theta_0\theta_3 + 2\theta_1\theta_2 + 2\theta_1\theta_3 + 2\theta_2\theta_3 \\
\end{align*}
\]

In actual applications, there are cases where the level coding has not essential meaning, such as for the designs of qualitative factors. However, for our purpose of solving a
system of polynomial equations using computational algebraic software, an appropriate level coding is important in view of computational time. In the author’s experiences, it is better to code \( \{-1,1\} \) rather than \( \{0,1\} \) for two-level factor, and \( \{-1,0,1\} \) rather than \( \{0,1,2\} \) for three-level factor. \( \square \)

As we see in Example \( 3.2 \), the relation (8) is very complicated compared to the relation for two-level cases (2). Among the various characterizations of the coefficients of the indicator functions of two-level designs given in [5], the relation of the indicator functions of complementary designs can be generalized to multilevel cases as follows.

**Proposition 3.3** (Generalization of Corollary 3.5 of [5]). If \( F \) and \( \bar{F} \) are complementary fractions and \( \theta = (\theta_a)_{a \in L} \) and \( \bar{\theta} = (\bar{\theta}_a)_{a \in L} \) are the coefficients of the corresponding indicator functions given by (3) respectively, then

\[
\theta_{0\ldots0} = 1 - \bar{\theta}_{0\ldots0} \quad \text{and} \quad \theta_a = -\bar{\theta}_a, \quad \forall \ a \neq (0\ldots,0).
\]

**Proof.** Write the model matrix \( X \) as

\[
X = \begin{bmatrix} 1_m & s_2 & \cdots & s_m \end{bmatrix}
\]

and write \( X^{-1}1_m = (c_1,\ldots,c_m)^T \). Then we have \( c_1 = 1, \ c_2 = \cdots = c_m = 0 \) from the non-singularity of \( X \) in the relation

\[
1_m = c_11_m + c_2s_2 + \cdots + c_ms_m.
\]

Therefore for the responses \( y, \bar{y} \in \{0,1\}^m \) such that \( y + \bar{y} = 1_m \), we have

\[
\theta + \bar{\theta} = X^{-1}(y + \bar{y}) = (1,0,\ldots,0)^T.
\]

\( \square \)

Next consider structure of the indicator functions of designs with given characteristic. We express the structure of the indicator functions as additional constraints to the system of polynomial equations (8) to classify designs with given characteristic. The additional constraints are derived as follows. Recall that the coefficients vector \( \theta \) is given by \( \theta = X^{-1}y \) in (3). Here, treat \( y = (y_i)_{i \in I} \) as a vector of \( \{0,1\}^m \) in (3) and express the characteristic of designs as

\[
c^Ty = s, \quad s \in \mathbb{Q}
\]

for a constant column vector \( c \in \mathbb{Q}^m \). For example, \( y \in \{0,1\}^m \) corresponding to designs with the size \( s \) satisfies the constraint

\[
1_m^Ty = s,
\]

where \( 1_m = (1,\ldots,1)^T \) is an \( m \times 1 \) column vector of the elements 1’s. Equireplicated designs or orthogonal designs can be expressed by

\[
c^Ty = 0
\]
for some contrast vectors $c$.

To make the arguments clear, we define a contrast matrix below. In the following definition, for each subset $J \subseteq [n]$ and index $i = (i_1, \ldots, i_n) \in \mathcal{I}$, we define $i_J$ by the restriction of $i$ to the index of $\prod_{j \in J} [r_j]$. For example of $n = 4$ and $J = \{1, 2, 4\}$, we have $i_J = (i_1, i_2, i_4)$. We also write $J = (j_1, J_2)$ and $\tilde{i} = (\tilde{i}_1, \tilde{i}_2)$ to separate the first element of $J$ and $\tilde{i}$, respectively.

**Definition 3.4.** The contrast matrix $C$ is an $m \times m$ matrix of the form

$$C^T = \begin{bmatrix} 1_m & C_1^T & C_2^T & \cdots & C_n^T \end{bmatrix},$$

where $C_k$ is a $v_k \times m$ matrix where

$$v_k = \sum_{J \subseteq [n], \#I = k} \left( \prod_{j \in J} (r_j - 1) \right).$$

The set of $m \times 1$ column vectors of $C_k^T$ is

$$\left\{ c_{J(\tilde{i})} = \{ c_{J(\tilde{i})}(i) \}_{i \in \mathcal{I}} : J \subseteq [n], \#J = k, \tilde{i} \in \prod_{j \in J} [r_j - 1] \right\},$$

where

$$c_{J(\tilde{i})}(i) = \begin{cases} 1, & i_J = 1, \\ -1, & i_J = \tilde{i} + 1, \\ 0, & \text{otherwise} \end{cases}$$

for $\#J = 1$, and

$$c_{J(\tilde{i})}(i) = \begin{cases} c_{J(\tilde{i})(2)}(i), & \text{if } i_{j_1} = \tilde{i}_1, \\ 0, & \text{otherwise} \end{cases}$$

for $\#J \geq 2$.

**Example 3.5** (Continuation of Example 3.2). For $2 \times 2 \times 3$ designs, the contrast matrix $C$ is given in Figure 4. Note that the contrast matrix $C$ is constructed only from $\mathcal{I}$, and does not depend on the level coding. □

By the contrast matrix, we specify the size and the orthogonality of the designs as follows. We call a design $F \subset D$ is orthogonal of strength $t$ ($t \leq n$), if for any $t$ factors, all possible combinations of levels appear equally often in $F$. This definition is from the theory of orthogonal arrays. See Chapter 7 of [11], for example. In particular, an orthogonal design of strength $n$ is a full factorial design.

**Proposition 3.6.** If $y \in \{0, 1\}^m$ is a response on $D$ given by (2), the fractional factorial design $F = \{ d_i \in D : i \in \mathcal{T}' \}$ is size $s$ and orthogonal of strength $t$ if and only if

$$Cy = \begin{bmatrix} 1_m y \\ C_1 y \\ \vdots \\ C_{t+1} y \\ C_m y \end{bmatrix} = \begin{bmatrix} s \\ 0_{v_1} \\ \vdots \\ 0_{v_t} \\ \ast \\ \vdots \\ \ast \end{bmatrix}$$
where $0_\ell = (0, \ldots, 0)^T$ is an $\ell \times 1$ column vector of the elements 0's.

**Proof.** Straightforward from Definition 3.4. □

From Proposition 3.6 and the relation $\theta = X^{-1}y$, the constraints to be added to the relation (8) for the orthogonal designs of strength $t \ (t \leq n)$ becomes

$$1_{m^T}X\theta = s, \ C_\ell X\theta = 0_{\ell r}, \ \ell = 1, \ldots, t.$$ 

This is a generalization of relation for two-level case such as (3).

**Example 3.7** (Continuation of Example 3.5). Consider $\{-1, 1\} \times \{-1, 1\} \times \{-1, 0, 1\}$ designs. In addition to the polynomial equations derived in Example 3.5, the coefficients of the indicator functions of designs with size $s$ satisfy the relation

$$12\theta_{000} + 8\theta_{002} = s.$$ 

The constraints for the equireplicated designs, i.e., orthogonal designs of strength 1, are

$$-12\theta_{100} - 8\theta_{102} = 0,$$
$$-12\theta_{010} - 8\theta_{012} = 0,$$
$$-4\theta_{001} + 4\theta_{002} = 0,$$
$$-8\theta_{001} = 0.$$ 

Therefore for a given $s$, we can enumerate all the equireplicated designs as the solutions of a system of these polynomial equations. □

**Remark 3.8.** The contrast matrix $C$ given in Definition 3.4 relates to theory of contingency tables. Suppose the response $y$ is a vector of nonnegative integers, then we can
treat \( y \) as a frequency of contingency table \( y = \{ y_i : i \in I \} \) with the set of cells \( I \). In this case, the condition
\[
1^T_m y = s, \ C \ell y = 0_{\ell t}, \ \ell = 1, \ldots, t,
\]
means equal \( \ell \)-dimensional marginal totals for \( \ell = 1, \ldots, t \). As another relation, \( C \) is a configuration matrix in the theory of toric ideals. See Section 1.5.3 of [7]. Anyway, there are several choices to define a contrast matrix \( C \) satisfying Proposition 3.6.

Now we give another representation of the indicator function reflecting the orthogonality. For the indicator function (5), consider a non-singular linear transformation \( \theta \mapsto \mu = CX \theta \). New variables \( z \) is also defined by \( z = ((CX)^{-1})^T x \). Then we have a representation of the indicator function for \( z = \{ z_{J(\tilde{i})} : J \subset [n], \tilde{i} \in \prod_{j \in J} [r_j - 1] \} \),
\[
f(z) = \sum_{J \subset [n], \tilde{i} \in \prod_{j \in J} [r_j - 1]} \mu_{J(\tilde{i})} z_{J(\tilde{i})}.
\]
(10)
We call (10) a contrast representation of the indicator function.

From the contrast representation, we see the size and the orthogonality of the designs directly, which is the advantage of the contrast representation. For example, the constant term \( \mu_{\emptyset} \) is the size of the design, and
\[
\mu_{J(\tilde{i})} = 0 \text{ for } \# J = 1, \tilde{i} \in \prod_{j \in J} [r_j - 1]
\]
corresponds to equireplicated designs, and so on.

**Example 3.9.** In Section 1, we see the indicator function of 34−2 regular fractional factorial design \( F_3 \) in Figure 2 is (4). The contrast representation of \( F_3 \) is
\[
f(z) = 9 + z_{123(111)} + z_{123(112)} - z_{123(122)} - z_{123(212)} - z_{123(221)} - z_{24(111)}
- z_{124(122)} + z_{124(212)} + z_{124(221)} - 2z_{134(111)} + 2z_{134(121)}
+ 2z_{134(122)} - z_{134(122)} - z_{134(212)} - z_{134(221)} - 2z_{234(111)} - z_{234(122)}
+ z_{234(212)} - z_{234(221)} - z_{234(111)} - z_{234(2221)}.
\]
From this representation, we see that the size of \( F_3 \) is 9, and \( F_3 \) is an orthogonal design of strength 2.

Another example is a 1/2 fraction of 2 × 2 × 3 design \( F_4 \) displayed in Figure 5. The indicator function and the contrast representation of \( F_4 \) are
\[
f(x_1, x_2, x_3) = \frac{1}{2} - \frac{1}{2} x_1 x_2 - \frac{1}{4} x_2 x_3 - \frac{1}{4} x_1 x_2 x_3 - \frac{1}{4} x_2 x_3^2 + 3 x_1 x_2 x_3^2
\]
(11)
and
\[
f(z) = 6 + 2z_{2(1)} + z_{12(11)} - z_{23(12)} + z_{123(111)},
\]
(12)
respectively. From the contrast representation, we see that the size of \( F_4 \) is 6. We also see that \( x_1 \) and \( x_3 \) are orthogonal from
\[
\mu_{1(1)} = \mu_{3(1)} = \mu_{3(2)} = \mu_{13(11)} = \mu_{13(12)} = 0.
\]
On the other hand, \( \mu_{2(1)} \neq 0 \) implies that \( F_3 \) is not equireplicated for \( x_2 \).
Figure 5: An example of $1/2$ fraction of $\{-1, 1\}^2 \times \{-1, 0, 1\}$ design.

Solving a system of polynomial equations for the coefficients of the indicator function or the contrast representation by computational algebraic softwares, we can obtain the complete list of fractional factorial designs with given orthogonality in theory. It is true that the computational feasibility is an important issue, which we see in Section 4. Another important point arises in classifying the solutions to the equivalence classes for permutations of levels or factors. For two-level cases, as we see in [5], the equivalence classes for permutations of levels and factors are simply obtained by sign changes or permutation of indices for the coefficients of the indicator functions. To consider multilevel cases, we give the description of the equivalence classes as follows. Suppose $S_\mathcal{I}$ is a group of permutations of $\mathcal{I}$, and $G \subseteq S_\mathcal{I}$ is a group we consider, i.e., a group of permutations of levels for each factor and permutations of factors if possible. For each $g \in G$, let $P_g$ be an $m \times m$ permutation matrix. Then the equivalence classes for $\theta$ and $\mu$ are

$$[\theta] = \{X^{-1}P_gX\theta : g \in G\}$$

and

$$[\mu] = \{C P_g C^{-1} \mu : g \in G\},$$

respectively.

**Example 3.10** (Continuation of Example 3.9). In Example 3.9, we see that the indicator function and the contrast representation of the $1/2$ fraction of $2 \times 2 \times 3$ design $F_4$ are (11) and (12), respectively. To see that the indicator functions and the contrast representations of the designs in the same equivalence class cannot be obtained only by sign changes or permutation of indices of (11) or (12), we illustrate all the elements in the equivalence class including $F_4$. Here, as a group $G \subseteq S_\mathcal{I}$, we consider the group of permutations of levels for each factor. Then we have $G = \langle e, g_1, g_2, g_{31}, g_{32} \rangle$, where

$$P_e = I_{12}, \ P_{g_1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes I_2 \otimes I_3, \ P_{g_2} = I_2 \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes I_3,$$

$$P_{g_{31}} = I_2 \otimes I_2 \otimes \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \ P_{g_{32}} = I_2 \otimes I_2 \otimes \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$I_k$ is a $k \times k$ identity matrix and $\otimes$ is a Kronecker product. For this group action, there are 12 relations in the same equivalence class belonging to $F_4$ displayed in Table 1.

\[\square\]
Table 1: Equivalence class including $F_4$. Upper: indicator functions, Lower: contrast representations. The coefficients not included in the table are 0.

| Design | $\theta_a$ | 000 | 010 | 110 | 011 | 111 | 012 | 112 |
|--------|------------|-----|-----|-----|-----|-----|-----|-----|
| $F_4$  | $\frac{1}{2}$ | 0   | $-\frac{1}{2}$ | $-\frac{1}{4}$ | $-\frac{1}{4}$ | $-\frac{1}{4}$ | 3/4 |
| No. 1  | $\frac{1}{2}$ | 0   | $\frac{1}{2}$  | $-\frac{1}{4}$ | $\frac{1}{4}$  | $-\frac{1}{4}$ | $-\frac{3}{4}$ |
| No. 2  | $\frac{1}{2}$ | 0   | $\frac{1}{2}$  | $\frac{1}{4}$  | $\frac{1}{4}$  | $\frac{1}{4}$  | $-\frac{3}{4}$ |
| No. 3  | $\frac{1}{2}$ | 0   | $\frac{1}{2}$  | $\frac{1}{4}$  | $-\frac{1}{4}$ | $-\frac{1}{4}$ | $-\frac{3}{4}$ |
| No. 4  | $\frac{1}{2}$ | 0   | $-\frac{1}{2}$ | $\frac{1}{4}$  | $\frac{1}{4}$  | $-\frac{1}{4}$ | 3/4  |
| No. 5  | $\frac{1}{2}$ | 0   | $-\frac{1}{2}$ | $\frac{1}{4}$  | $-\frac{1}{4}$ | $\frac{1}{4}$  | 3/4  |
| No. 6  | $\frac{1}{2}$ | 0   | $\frac{1}{2}$  | $-\frac{1}{4}$ | $-\frac{1}{4}$ | $\frac{1}{4}$  | $-\frac{3}{4}$ |
| No. 7  | $\frac{1}{2}$ | 0   | $-\frac{1}{2}$ | $-\frac{1}{4}$ | $\frac{1}{4}$  | $\frac{1}{4}$  | 3/4  |
| No. 8  | $\frac{1}{2}$ | $-\frac{1}{2}$ | 0   | 0   | $\frac{1}{2}$ | $\frac{1}{2}$  | 0    |
| No. 9  | $\frac{1}{2}$ | $-\frac{1}{2}$ | 0   | 0   | $-\frac{1}{2}$ | $\frac{1}{2}$  | 0    |
| No. 10 | $\frac{1}{2}$ | $\frac{1}{2}$ | 0   | 0   | $-\frac{1}{2}$ | $-\frac{1}{2}$ | 0    |
| No. 11 | $\frac{1}{2}$ | $\frac{1}{2}$ | 0   | 0   | $\frac{1}{2}$ | $-\frac{1}{2}$ | 0    |

| Design | $\mu_{J(i)}$ | Const | 2(1) | 12(11) | 23(11) | 23(12) | 123(111) | 123(112) |
|--------|--------------|-------|------|--------|--------|--------|-----------|-----------|
| $F_4$  | 6            | 2     | 1    | 0      | $-1$   | 1      | 1         | 0         |
| No. 1  | 6            | 2     | 1    | 0      | $-1$   | 1      | $-1$      | 0         |
| No. 2  | 6            | $-2$  | 1    | 1      | 1      | 0      | 1         | 0         |
| No. 3  | 6            | 2     | $-2$ | 1      | 1      | 1      | 0         | 1         |
| No. 4  | 6            | 2     | 1    | 1      | 1      | 1      | 0         | 1         |
| No. 5  | 6            | $-2$  | 1    | 1      | 0      | 1      | 1         | 1         |
| No. 6  | 6            | $-2$  | $-1$ | 1      | 1      | $-1$   | 0         | $-1$      |
| No. 7  | 6            | $-2$  | $-1$ | $-1$   | 1      | $-1$   | 0         | $-1$      |
| No. 8  | 6            | 2     | 1    | $-1$   | 0      | $-1$   | $-1$      | 0         |
| No. 9  | 6            | 2     | 1    | $-1$   | 0      | 0      | 1         | 1         |
| No. 10 | 6            | $-2$  | $-1$ | 1      | 0      | 1      | 1         | 1         |
| No. 11 | 6            | $-2$  | $-1$ | 1      | 0      | 0      | 0         | $-1$      |
4 Classifications of orthogonal $2^3 \times 3$ and $2^4 \times 3$ designs

In this section, we consider $2^3 \times 3$ and $2^4 \times 3$ designs. Using a computational algebraic software, we solve systems of the polynomial equations and derive a classification of designs with given characteristic. All the computations are done by Macaulay2 ([G]) installed in a virtual machine (vmware) on a laptop with 2.80 GHz CPU and 8 GB memory. The memory allocated to the virtual machine is 512 MB.

4.1 Full enumeration of the orthogonal fractions of the $2^3 \times 3$ designs of strength 2

First we consider the orthogonal fractions of the $2^3 \times 3$ designs of strength 2. Corresponding system of algebraic equations includes a set of $m = 2^3 \times 3 = 24$ general relations, 1 relation for the size, 5 relations for the balance for each factor and 9 relations for the orthogonality of strength 2, for 25 variables. Note that there are $m + 1$ variables, where $+1$ corresponds to the variable for the size $s$. To obtain a compatible size $s$, first we calculate the Gröbner basis of the ideal $I$ generated by the 39 polynomials corresponding to the above 39 relations for the elimination ordering where the variable $s$ is the lowest. The Gröbner basis is calculated within 0.1 seconds, and the elimination ideal is

$$ I \cap \mathbb{Q}[s] = \langle s^3 - 36s^2 + 288s \rangle = \langle s(s - 12)(s - 24) \rangle, $$

i.e., only the size $s = 12$ is compatible. This result is also obvious because the size of the orthogonal designs must be the multiple of $2 \times 2$ and $2 \times 3$. Therefore we fix $s = 12$ and calculate all the solutions. We find that there are 44 solutions, classified into 3 equivalence classes as follows.

- Type (a): 2 relations. The indicator function and the contrast representation of the representative fraction displayed in Figure 6(a) are

$$ \frac{1}{2} + \frac{1}{2}x_1x_2x_3 $$

and

$$ 12 - 3z_{123(111)}, $$

respectively. This is a class of the regular fractional factorial designs with the defining relation $x_1x_2x_3 = 1$.

- Type (b): 6 relations. The indicator function and the contrast representation of the representative fraction displayed in Figure 6(b) are

$$ \frac{1}{2} + \frac{1}{2}x_1x_2x_3 - \frac{1}{2}x_1x_2x_3x_4 - \frac{1}{2}x_1x_2x_3x_4^2 $$

and

$$ 12 - z_{123(111)} - z_{1234(1112)}, $$
respectively, each with 4 relations. The indicator function and the contrast representation of another fraction in the same equivalence class are

\[ \frac{1}{2} - \frac{1}{2} x_1 x_2 x_3 + x_1 x_2 x_3 x_4^2 \]

and

\[ 12 - z_{123(111)} - z_{1234(1111)} \]

respectively, each with 2 relations.

• Type (c): 36 relations. The indicator function and the contrast representation of the representative fraction displayed in Figure 6(c) are

\[ \frac{1}{2} + \frac{1}{2} x_1 x_2 x_3 - \frac{1}{2} x_1 x_3 x_4 - \frac{1}{2} x_1 x_2 x_3 x_4^2 \]

and

\[ 12 - z_{123(111)} + z_{134(111)} + 2z_{134(112)} + z_{1234(1111)} + z_{1234(1112)} \]

respectively, each with 12 relations. The indicator function and the contrast representation of another fraction in the same equivalence class are

\[ \frac{1}{2} - \frac{1}{2} x_1 x_2 - \frac{1}{4} x_1 x_2 x_4 + \frac{1}{4} x_1 x_2 x_3 x_4 + \frac{3}{4} x_1 x_2 x_4^2 + \frac{1}{4} x_1 x_2 x_3 x_4^2 \]

and

\[ 12 - z_{123(111)} + 2z_{124(111)} + z_{124(112)} + z_{1234(1111)} + z_{1234(1112)} \]

respectively, each with 24 relations.

| Type(a) | Type(b) | Type(c) |
|---------|---------|---------|
| \( x_1 \) | \( x_2 \) | \( x_3 \) | \( x_4 \) |
| 1 1 1 -1 | 1 1 1 -1 | 1 1 1 -1 |
| 1 1 1 0 | 1 1 1 0 | 1 1 1 0 |
| 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 0 | 1 -1 -1 0 | 1 -1 -1 0 |
| 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 0 | -1 1 -1 0 | -1 1 -1 0 |
| -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 0 | -1 -1 1 0 | -1 -1 1 0 |
| -1 -1 1 1 | -1 -1 -1 1 | -1 -1 -1 1 |

Figure 6: Orthogonal fractions of the \( 2^3 \times 3 \) designs of strength 2

In the above list, Type (a) is the class of the regular fractions, whereas Type (b) and Type (c) are classes of the non-regular fractions. Note that Type (b) and Type (c)
differ only in the last columns (the levels of $x_4$) in Figure 6. For each row where the levels of $(x_1, x_2, x_3)$ is unique, there are 4 such rows, the levels of $x_4$ are fixed ($x_4 = 1$) in Type (b), whereas the levels of $x_4$ are 1 or $-1$ in Type (c). Type (b) and (c) can also be characterized considering the designs obtained from a traditional $OA(12, 3^12^4)$ orthogonal array as follows. The orthogonal array $OA(12, 3^12^4)$ in Appendix 8C of [11] is displayed in Figure 7. From $OA(12, 3^12^4)$, we can obtain 1/2 fractions of $2^3 \times 3$ designs by selecting 3 columns from the columns $\{2, 3, 4, 5\}$. We see that all the designs constructed in this way are included in the equivalence class of Type (c). Therefore Type (c) is regarded as the class of $OA(12, 3^12^4)$ designs.

4.2 Full enumeration of the orthogonal fractions of the $2^4 \times 3$ designs of strength 3

Next we consider the fractions of the $2^4 \times 3$ designs. For this case, enumeration of the orthogonal fractions of strength 2 may be difficult to compute for standard PC. In fact, the Gröbner basis of the elimination ideal for the compatible size does not obtained after 1 week calculation. Therefore we enumerate the orthogonal fractions of strength 3 instead. Note that, for fixed size $s$, there are $m = 48$ variables with constraints $1 + 6 + 14 = 21$ relations for strength 2, and with constraints $1 + 6 + 14 + 16 = 37$ relations for strength 3. Therefore, by eliminating variables, the number of variables reduces 11 for strength 3, whereas to 27 for strength 2. The compatible size must be $s = 24$ for strength 3, that is only the multiple of $2 \times 2 \times 2$ and $2 \times 2 \times 3$ less than $m = 48$. This fact is also checked by the Gröbner basis calculation. After calculation within 0.1 seconds, we see that the elimination ideal is

$$I \cap \mathbb{Q}[s] = \langle s^3 - 72s^2 + 1152s \rangle = \langle s(s-24)(s-48) \rangle.$$

Therefore we fix $s = 24$ and calculate all the solutions. We find there are 56 solutions, classified into 3 equivalence classes as follows.

$$
\begin{array}{ccccc}
1 & 2 & 3 & 4 & 5 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 1 & 1 \\
0 & 1 & 1 & 1 & 0 \\
1 & 0 & 0 & 1 & 1 \\
1 & 0 & 1 & 1 & 0 \\
1 & 1 & 0 & 0 & 1 \\
1 & 1 & 1 & 0 & 0 \\
2 & 0 & 0 & 1 & 0 \\
2 & 0 & 1 & 0 & 1 \\
2 & 1 & 0 & 0 & 0 \\
2 & 1 & 1 & 1 & 1 \\
\end{array}
$$

Figure 7: Orthogonal array $OA(12, 3^12^4)$ (Appendix 8C of [11]).
• Type (a): 2 relations. The indicator function and the contrast representation of the representative fraction displayed in Figure 8(a) are
\[ \frac{1}{2} + \frac{1}{2}x_1x_2x_3x_4 \]
and
\[ 24 + 3z_{1234(1111)}, \]
respectively. This is a class of the regular fractional factorial designs with the defining relation \( x_1x_2x_3x_4 = 1 \).

• Type (b): 6 relations. The indicator function and the contrast representation of the representative fraction displayed in Figure 8(b) are
\[ \frac{1}{2} - \frac{1}{2}x_1x_2x_3x_4 - \frac{1}{2}x_1x_2x_3x_4x_5 + \frac{1}{2}x_1x_2x_3x_4x_5^2 \]
and
\[ 24 - z_{1234(1111)} + z_{12345(11111)} + z_{12345(11112)}, \]
respectively, each with 4 relations. The indicator function and the contrast representation of another fraction in the same equivalence class are
\[ \frac{1}{2} + \frac{1}{2}x_1x_2x_3x_4 - x_1x_2x_3x_4x_5^2 \]
and
\[ 24 - z_{1234(1111)} - z_{12345(11111)}, \]
respectively, each with 2 relations.

• Type (c): 48 relations. The indicator function and the contrast representation of the representative fraction displayed in Figure 8(c) are
\[ \frac{1}{2} - \frac{1}{2}x_1x_2x_3x_4 - \frac{1}{2}x_1x_2x_3x_4x_5 + \frac{1}{2}x_1x_2x_3x_4x_5^2 \]
and
\[ 24 - z_{1234(1111)} - z_{1245(11111)} - 2z_{1245(11112)} - z_{12345(11112)}, \]
respectively, each with 16 relations. The indicator function and the contrast representation of another fraction in the same equivalence class are
\[ \frac{1}{2} + \frac{1}{2}x_1x_2x_3 + \frac{1}{4}x_1x_2x_3x_5 + \frac{1}{4}x_1x_2x_3x_4x_5 - \frac{3}{4}x_1x_2x_3x_5^2 + \frac{1}{4}x_1x_2x_3x_4x_5^2 \]
and
\[ 24 + z_{1234(1111)} + 2z_{1235(11111)} + z_{1235(11112)} + z_{12345(11111)}, \]
respectively, each with 32 relations.

An interpretation of this list is similar to the \( 2^3 \times 3 \) case. In Figure 8 Type (b) and Type (c) differ only in the last column (the levels of \( x_5 \)). For each row where the levels of \( (x_1, x_2, x_3, x_4) \) is unique, there are 8 such rows, the levels of \( x_5 \) are fixed \( (x_5 = -1) \) in Type (b), whereas the levels of \( x_5 \) are 1 or \(-1\) in Type (c).
| Type(a) | Type(b) | Type(c) |
|---------|---------|---------|
| $x_1$  | $x_2$  | $x_3$  | $x_4$  | $x_5$ | $x_1$  | $x_2$  | $x_3$  | $x_4$  | $x_5$ | $x_1$  | $x_2$  | $x_3$  | $x_4$  | $x_5$ |
| $-1$   | $-1$   | $-1$   | $-1$   | $1$    | $-1$   | $-1$   | $-1$   | $1$    | $0$   | $-1$   | $-1$   | $-1$   | $1$    | $1$    |
| $-1$   | $-1$   | $-1$   | $0$    | $-1$   | $-1$   | $-1$   | $1$    | $1$    | $1$   | $-1$   | $-1$   | $-1$   | $0$    | $-1$   |
| $-1$   | $-1$   | $1$    | $1$    | $-1$   | $0$    | $-1$   | $1$    | $-1$   | $1$   | $-1$   | $1$    | $1$    | $1$    | $1$    |
| $0$    | $-1$   | $1$    | $1$    | $-1$   | $1$    | $-1$   | $-1$   | $1$    | $1$   | $-1$   | $1$    | $1$    | $-1$   | $-1$   |
| $1$    | $1$    | $1$    | $-1$   | $1$    | $-1$   | $1$    | $1$    | $1$    | $1$   | $-1$   | $1$    | $1$    | $1$    | $1$    |
| $1$    | $1$    | $1$    | $1$    | $1$    | $-1$   | $1$    | $1$    | $1$    | $1$   | $1$    | $1$    | $1$    | $1$    | $1$    |
| $1$    | $-1$   | $1$    | $-1$   | $1$    | $-1$   | $1$    | $1$    | $1$    | $0$   | $1$    | $-1$   | $1$    | $-1$   | $-1$   |
| $1$    | $1$    | $1$    | $1$    | $1$    | $1$    | $1$    | $1$    | $0$    | $-1$  | $1$    | $1$    | $1$    | $1$    | $1$    |
| $1$    | $-1$   | $1$    | $-1$   | $1$    | $1$    | $1$    | $1$    | $0$    | $-1$  | $1$    | $1$    | $1$    | $-1$   | $-1$   |
| $1$    | $1$    | $1$    | $1$    | $1$    | $1$    | $1$    | $1$    | $1$    | $1$   | $-1$   | $1$    | $1$    | $0$    | $-1$   |
| $1$    | $1$    | $1$    | $1$    | $1$    | $-1$   | $1$    | $1$    | $0$    | $-1$  | $1$    | $1$    | $1$    | $-1$   | $-1$   |
| $1$    | $1$    | $1$    | $1$    | $-1$   | $1$    | $1$    | $1$    | $0$    | $-1$  | $1$    | $1$    | $1$    | $-1$   | $-1$   |
| $1$    | $1$    | $1$    | $0$    | $-1$   | $1$    | $1$    | $0$    | $-1$   | $1$   | $-1$   | $1$    | $1$    | $1$    | $1$    |
| $1$    | $1$    | $1$    | $-1$   | $1$    | $1$    | $1$    | $1$    | $0$    | $-1$  | $1$    | $1$    | $1$    | $-1$   | $-1$   |

Figure 8: Orthogonal fractions of the $2^4 \times 3$ designs of strength 3
5 Discussion

In this paper, we give how to construct a system of polynomial equations for the coefficients of the indicator functions of multi-level fractional factorial designs with given orthogonality. We also define the contrast representation of the indicator function, which reflects the orthogonality of the design directly. Using these results, we show the classifications of the orthogonal fractions of the $2^3 \times 3$ designs with strength 2 and $2^4 \times 3$ designs with strength 3.

In theory, we can obtain classifications of fractional factorial designs for any size by our method. However, the computational feasibility depends on the size of problems. For the class of $2^m \times 3$ designs, we see that the $2^4 \times 3$ problem for orthogonality with strength 3 is easy to calculate. However, a $2^5 \times 3$ problem of strength 3 orthogonality seems very difficult to compute. As for the class of $2^m \times 3^2$ designs, we find that the $2^3 \times 3^2$ problem of strength 2 orthogonality is hard to compute, i.e., the Gröbner basis calculation for the elimination ideal does not finish in 1 week. In addition, it is obvious that there is no orthogonal fractions $2^3 \times 3^2$ with strength 3 because the size must be a multiple of $2 \times 2 \times 2$ and $2 \times 3 \times 3$. As a consequence, we only have limited computational results in this paper.

In particular, the merit of the contrast representation must be investigated from the computational aspects. It seems that a system of polynomial equations for $\mu$ is easy to solve than that for $\theta$. Note that the polynomial relations for $\mu$ are obtained by substituting $\theta = (CX)^{-1}\mu$ to the polynomial relations for $\theta$. Therefore, translating the relations for $\theta$ to the relations for $\mu$ corresponds to the matrix operations of inverse in advance. Unfortunately, for the problems considered in this paper, the systems of the polynomial equations for $\theta$ and $\mu$ are both quite easy or quite difficult, and the effectiveness of the contrast representation from the computational aspect is not shown. Therefore the quantitative evaluation of the effect of this transformation is one of the open problems.

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