

Indicator Functions and the Algebra of the Linear-Quadratic Parametrization

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SUMMARY

Indicator functions are constructed under the linear-quadratic parametrization for contrasts, and applied to the study of partial aliasing properties for three-level fractional factorial designs. An algebraic operation is introduced for the calculation of indicator function coefficients. This operation connects design construction methods to the analysis under the linear-quadratic system, and helps establish simple conditions for the estimability of interactions.

Some key words: Fractional factorial design; Generator-transformation design; Partial aliasing.

1. INTRODUCTION

1.1. *The utility of the linear-quadratic parametrization*

Fractional factorial designs help address the challenge of screening and estimating main effects and interactions simultaneously for experiments with many factors and run size constraints. An important issue in their construction and subsequent analysis is the parametrization for factorial effects. The orthogonal components system (Wu & Hamada, 2009, p. 274) is a standard parametrization that facilitates calculations of design properties for regular fractions. However, it has two major disadvantages: it can induce a simple aliasing structure, with any two contrasts either perfectly correlated or orthogonal (Ye, 2004), and it does not yield substantive interpretations for interaction components of quantitative factors.

These facts are illustrated in the example of a 3_{IV}^{4-1} design with quantitative factors (Wu & Hamada, 2009, p. 267–269, 281). If a pair of aliased two-factor interactions is judged significant in its orthogonal components analysis, then conclusive inferences on specific interactions cannot be made without further runs. One alternative system that does yield conclusive inferences and interpretable contrasts is the linear-quadratic system, generated by reparametrizing the factor levels using orthogonal polynomials (Wu & Hamada, 2009, p. 61, 287–288). The capacity for estimating two-factor interactions is better under the linear-quadratic system (Wu & Hamada, 2009, p. 292–293) because they are only partially aliased, in the sense that the absolute correlation of any pair of two-factor interaction contrasts is strictly less than 1. Although this design is regular, i.e., constructed by aliasing relations in a finite field, the linear-quadratic system yields

a nonregular analysis through the introduction of partial aliasing. This enables a sequential strategy for de-aliasing factorial effects and identifying significant interactions that would otherwise be missed, with no need for further runs (Hamada & Wu, 1992; Wu & Hamada, 2009, p. 292). For all these reasons, the linear-quadratic system is preferable to orthogonal components.

However, the mathematics of the linear-quadratic system are not yet as transparent as the field theory basis for orthogonal components. A better understanding of the partial aliasing properties of this system is achieved with the indicator function of a design, and the focus of the current paper is to further develop the theory of indicator functions under the linear-quadratic system.

1.2. Previous applications of indicator functions

Based on the algebraic perspective of Pistone & Wynn (1996), Fontana et al. (2000) introduced the indicator function of unreplicated two-level fractional factorials, and proved the important fact that indicator function coefficients describe correlations between contrasts. Both Ye (2004) and Pistone & Rogantin (2008) considered indicator functions for designs with factors having more than two levels, but coded the levels by the complex roots of unity. A complex coding may be concise and amenable for generalizations to different settings, but we instead code factor levels with orthogonal polynomials, which may ultimately be used when fitting a model for the response, e.g., as in response surface methodology. Cheng & Ye (2004) considered indicator functions under the linear-quadratic system, and defined the concept of geometric isomorphism to consider changes in design properties corresponding to permutations in factor levels.

2. INDICATOR FUNCTIONS UNDER THE LINEAR-QUADRATIC PARAMETRIZATION

Let \mathcal{D} be a 3^s full factorial, with the levels of factors A_1, \dots, A_s denoted by $-1, 0, 1$, corresponding to $0, 1, 2$ modulo 3 in the standard field notation. Field theory succinctly describes certain designs, and so it is necessary to move between these two notations. For example, when translating the regular fraction in Table 1 into linear-quadratic notation, runs having A_1 at level 0 and A_2 at level 1 must have A_3 at level -1 in the linear-quadratic system, corresponding to $1 + 2 = 0$ modulo 3 in the field notation. It is also necessary to refer to orthogonal arrays having N runs, s factors, each with three levels, and strength t , and they are abbreviated as $\text{OA}(N, s, 3, t)$.

Table 1. *Design with $A_3 = A_1 + A_2$ modulo 3. Three columns on the left represent the design under field notation, and the three on the right represent it using linear-quadratic notation.*

Field Theory			Linear-Quadratic		
A_1	A_2	A_3	A_1	A_2	A_3
0	0	0	-1	-1	-1
0	1	1	-1	0	0
0	2	2	-1	1	1
1	0	1	0	-1	0
1	1	2	0	0	1
1	2	0	0	1	-1
2	0	2	1	-1	1
2	1	0	1	0	-1
2	2	1	1	1	0

The indicator function $F : \{-1, 0, 1\}^s \rightarrow \{0, 1\}$ for a fraction $\mathcal{F} \subseteq \mathcal{D}$ is the mapping with $F(x) = 1$ if $x \in \mathcal{F}$ and 0 otherwise, which can be extended for replicated runs using the generalized indicator function (Ye, 2003). This function is expressed as a unique linear combination

of orthogonal contrast functions under the linear-quadratic system (Cheng & Ye, 2004). For each $i \in \{1, \dots, s\}$, functions $X_{i,L}, X_{i,Q} : \mathbb{R}^s \rightarrow \mathbb{R}$ are defined as

$$X_{i,L}(x) = x_i, \quad X_{i,Q}(x) = 3x_i^2 - 2.$$

These correspond to linear and quadratic contrasts for the main effect of A_i (Wu & Hamada, 2009, p. 287). For distinct $i_1, \dots, i_k \in \{1, \dots, s\}$, and any $T_1, \dots, T_k \in \{L, Q\}$, define

$$X_{i_1 \dots i_k, T_1 \dots T_k}(x) = \prod_{j=1}^k X_{i_j, T_j}(x), \quad (1)$$

which corresponds to the $T_1 \dots T_k$ interaction contrast of A_{i_1}, \dots, A_{i_k} . Define $X_{\phi, \phi}(x) \equiv 1$, corresponding to the overall average. Functions $\{X_{I,T}(x) : I \in \mathcal{P}, T \in \mathcal{T}_I\}$ form an orthogonal basis for \mathcal{D} , where \mathcal{P} is the set of all concatenations of distinct elements from $\{1, \dots, s\}$, and \mathcal{T}_I is the set of all concatenations of $|I|$ elements from $\{L, Q\}$. This is summarized by the following lemma, given by Fontana et al. (2000) for two-level designs, and Cheng & Ye (2004).

LEMMA 1. For $I_1, I_2 \in \mathcal{P}$ and $T_1 \in \mathcal{T}_{I_1}, T_2 \in \mathcal{T}_{I_2}$, $\sum_{x \in \mathcal{D}} X_{I_1, T_1}(x) X_{I_2, T_2}(x) \neq 0$ if and only if $I_1 = I_2, T_1 = T_2$.

Lemma 1 implies that the indicator function is a unique linear combination of basis functions in (1): there exist unique $b_{I,T} \in \mathbb{R}$ for all $I \in \mathcal{P}, T \in \mathcal{T}_I$ such that

$$F(x) = \sum_{I \in \mathcal{P}} \sum_{T \in \mathcal{T}_I} b_{I,T} X_{I,T}(x). \quad (2)$$

Partial aliasing relations can be read from the indicator function coefficients $b_{I,T}$. The correlation of two contrasts having distinct factors is positively proportional to the coefficient involving all the factors, and correlations between contrasts involving the same factors are simple functions of these coefficients.

Calculation of the $b_{I,T}$ will be demonstrated later. At this point, the indicator function for the design in Table 1 is given to illustrate how representation (2) is connected to partial aliasing:

$$\begin{aligned} F(x) = & \frac{1}{3} - \frac{3}{8}x_1x_2x_3 - \frac{1}{8}x_1x_2(3x_3^2 - 2) + \frac{1}{8}x_1(3x_2^2 - 2)x_3 - \frac{1}{8}x_1(3x_2^2 - 2)(3x_3^2 - 2) \\ & + \frac{1}{8}(3x_1^2 - 2)x_2x_3 - \frac{1}{8}(3x_1^2 - 2)x_2(3x_3^2 - 2) + \frac{1}{8}(3x_1^2 - 2)(3x_2^2 - 2)x_3 \\ & + \frac{1}{24}(3x_1^2 - 2)(3x_2^2 - 2)(3x_3^2 - 2). \end{aligned}$$

Coefficients involving one or two factors are zero precisely because the involved contrasts are orthogonal in this design. For example, $b_{12,LL} = 0$ because the linear main effect of A_1 , denoted by $(A_1)_L$, is orthogonal to the linear main effect of A_2 , $(A_2)_L$. Alternatively, these coefficients are zero because the contrasts represented by these basis functions are valid, in the sense that they are orthogonal to the vector of ones. Thus, $b_{12,LL} = 0$ because the two-factor linear-linear interaction between A_1 and A_2 , i.e., the difference in the conditional linear effects of A_2 between the high and low levels of A_1 (Wu & Hamada, 2009, p. 288), denoted by $(A_1A_2)_{LL}$, is orthogonal to $(1, \dots, 1)' \in \mathbb{R}^9$. Also, the correlation between $(A_1A_2)_{LL}$ and $(A_3)_L$ is proportional to $b_{123,LLL} = -3/8$, and the correlation between $(A_1A_2)_{LL}$ and $(A_1A_3)_{LL}$ is proportional to $b_{123,QLL} + b_{23,LL} = 1/8$, with different, but positive, proportionality constants for both.

3. THE KRONECKER PRODUCT OPERATION ON FACTORS

Calculation of indicator function coefficients involving all linear effects is accomplished by Corollary 2.2 in (Cheng & Ye, 2004). The following proposition summarizes a new calculation for coefficients involving at least one quadratic effect. All proofs are in the appendix.

PROPOSITION 1. For distinct $i_1, \dots, i_k \in \{1, \dots, s\}$, and $T_1, \dots, T_k \in \{L, Q\}$ with $T_1, \dots, T_j = L, T_{j+1}, \dots, T_k = Q$, and $1 \leq j < k$, define

$$B_{i_1 \dots i_k, T_1 \dots T_k} = \begin{cases} b_{i_1 \dots i_j, T_1 \dots T_j}, & k = j + 1, \\ b_{i_1 \dots i_j, T_1 \dots T_j} + \sum_{m=1}^{k-j-1} \left(\sum_{\substack{l_1, \dots, l_m \in \{j+1, \dots, k\}: \\ l_1 < \dots < l_m}} b_{i_1 \dots i_j i_{l_1} \dots i_{l_m}, T_1 \dots T_j T_{l_1} \dots T_{l_m}} \right), & k > j + 1. \end{cases}$$

Then

$$b_{i_1 \dots i_k, T_1 \dots T_k} = 2^{-k} 3^{k-s} \sum_{x \in \mathcal{F}} X_{i_1, L}(x)^{a_1} \dots X_{i_k, L}(x)^{a_k} - B_{i_1 \dots i_k, T_1 \dots T_k}, \quad (3)$$

where $a_1 = \dots = a_j = 1$, and $a_{j+1} = \dots = a_k = 2$.

Also, define

$$B_{i_1 \dots i_k, Q \dots Q} = b_{\phi, \phi} + \sum_{m=1}^{k-1} \left(\sum_{\substack{l_1, \dots, l_m \in \{1, \dots, k\}: \\ l_1 < \dots < l_m}} b_{i_{l_1} \dots i_{l_m}, Q \dots Q} \right).$$

Then

$$b_{i_1 \dots i_k, Q \dots Q} = 2^{-k} 3^{k-s} \sum_{x \in \mathcal{F}} X_{i_1, L}(x)^2 \dots X_{i_k, L}(x)^2 - B_{i_1 \dots i_k, Q \dots Q}. \quad (4)$$

There are three points to note. First, Proposition 1 involves $b_{\phi, \phi} = |\mathcal{F}|/3^s$ (Cheng & Ye, 2004). Second, it connects low-order and high-order coefficients, and shows how factors with linear effects carry through. If a set of factors form an orthogonal array of strength t , then all coefficients involving t or fewer of these factors are zero. As described later, the combination of this fact with Proposition 1 illuminates calculations of a design's properties. Third, if interest lies in specific high-order coefficients, the calculation method of Cheng & Ye (2004, p. 2173) is better.

To demonstrate Proposition 1, consider Table 1. This is an orthogonal array of strength 2, so $b_{i_1, T_1} = b_{i_1 i_2, T_1 T_2} = 0$ for distinct $i_1, i_2 \in \{1, 2, 3\}$, and any $T_1, T_2 \in \{L, Q\}$. Then:

$$b_{123, LLQ} = \frac{1}{8} \sum_{x \in \mathcal{F}} X_{1, L}(x) X_{2, L}(x) X_{3, L}(x)^2 = -\frac{1}{8},$$

$$b_{123, LQQ} = \frac{1}{8} \sum_{x \in \mathcal{F}} X_{1, L}(x) X_{2, L}(x)^2 X_{3, L}(x)^2 = -\frac{1}{8},$$

$$b_{123, QQQ} = \frac{1}{8} \sum_{x \in \mathcal{F}} X_{1, L}(x)^2 X_{2, L}(x)^2 X_{3, L}(x)^2 - b_{\phi, \phi} = \frac{3}{8} - \frac{1}{3} = \frac{1}{24}.$$

This shows how Proposition 1 eliminates the need to deal with quadratic contrast functions.

Proposition 1 is used to define an operation for factors under the linear-quadratic system that enables one to read from the design in linear-quadratic notation to calculate the $b_{I,T}$. For any $i \in \{1, \dots, s\}$, define $\mathcal{F}_{i,L} = \{x \in \mathcal{F} : x_i = 1\}$, $\mathcal{F}_{i,Q} = \{x \in \mathcal{F} : x_i = -1\}$. By Proposition 1,

$$\begin{pmatrix} b_{i,L} \\ b_{i,Q} \end{pmatrix} = 2^{-1} 3^{1-s} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} |\mathcal{F}_{i,L}| \\ |\mathcal{F}_{i,Q}| \end{pmatrix} - \begin{pmatrix} 0 \\ b_{\phi,\phi} \end{pmatrix}.$$

Coefficients for factors A_{i_1} and A_{i_2} are then obtained by a scaled Kronecker product of Hadamard matrices, and an intersection of the sets defined above, again by Proposition 1. Specifically, defining $\mathcal{F}_{i_1 i_2, T_1 T_2} = \mathcal{F}_{i_1, T_1} \cap \mathcal{F}_{i_2, T_2}$ for any $T_1, T_2 \in \{L, Q\}$,

$$\begin{pmatrix} b_{i_1 i_2, LL} \\ b_{i_1 i_2, LQ} \\ b_{i_1 i_2, QL} \\ b_{i_1 i_2, QQ} \end{pmatrix} = 2^{-2} 3^{2-s} \left\{ \bigotimes_{j=1}^2 \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \right\} \begin{pmatrix} |\mathcal{F}_{i_1 i_2, LL}| \\ |\mathcal{F}_{i_1 i_2, LQ}| \\ |\mathcal{F}_{i_1 i_2, QL}| \\ |\mathcal{F}_{i_1 i_2, QQ}| \end{pmatrix} - \begin{pmatrix} 0 \\ B_{i_1 i_2, LQ} \\ B_{i_1 i_2, QL} \\ B_{i_1 i_2, QQ} \end{pmatrix}.$$

We formally define $A_{i_1} \otimes A_{i_2} = (b_{i_1 i_2, LL}, b_{i_1 i_2, LQ}, b_{i_1 i_2, QL}, b_{i_1 i_2, QQ})'$.

This operation is easily extended to more than two factors: $A_{i_1} \otimes \dots \otimes A_{i_k}$ is defined as the vector of indicator function coefficients, in a lexicographic ordering of linear and quadratic effects, involving all these k distinct factors. To write this explicitly, define

$$\mathcal{F}_{i_1 \dots i_k, T_1 \dots T_k} = \bigcap_{j=1}^k \mathcal{F}_{i_j, T_j}$$

for any $T_{i_1}, \dots, T_{i_k} \in \{L, Q\}$. Then, by Proposition 1,

$$A_{i_1} \otimes \dots \otimes A_{i_k} = 2^{-k} 3^{k-s} \left\{ \bigotimes_{j=1}^k \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \right\} \begin{pmatrix} |\mathcal{F}_{i_1 \dots i_{(k-1)} i_k, L \dots LL}| \\ |\mathcal{F}_{i_1 \dots i_{(k-1)} i_k, L \dots LQ}| \\ |\mathcal{F}_{i_1 \dots i_{(k-1)} i_k, L \dots QL}| \\ |\mathcal{F}_{i_1 \dots i_{(k-1)} i_k, L \dots QQ}| \\ \vdots \\ |\mathcal{F}_{i_1 \dots i_{(k-1)} i_k, Q \dots LL}| \\ |\mathcal{F}_{i_1 \dots i_{(k-1)} i_k, Q \dots LQ}| \\ |\mathcal{F}_{i_1 \dots i_{(k-1)} i_k, Q \dots QL}| \\ |\mathcal{F}_{i_1 \dots i_{(k-1)} i_k, Q \dots QQ}| \end{pmatrix} - \begin{pmatrix} 0 \\ B_{i_1 \dots i_{(k-1)} i_k, L \dots LQ} \\ B_{i_1 \dots i_{(k-1)} i_k, L \dots QL} \\ B_{i_1 \dots i_{(k-1)} i_k, L \dots QQ} \\ \vdots \\ B_{i_1 \dots i_{(k-1)} i_k, Q \dots LL} \\ B_{i_1 \dots i_{(k-1)} i_k, Q \dots LQ} \\ B_{i_1 \dots i_{(k-1)} i_k, Q \dots QL} \\ B_{i_1 \dots i_{(k-1)} i_k, Q \dots QQ} \end{pmatrix}.$$

Thus, counts of ± 1 level combinations are sufficient for calculating indicator function coefficients under the linear-quadratic system. Applying an affine transformation to these counts by first performing a scaled rotation, corresponding to the scaled Hadamard matrix built by the Kronecker product, and then a shift by coefficients of lower order, consisting of factors with linear effects and subsets of factors with quadratic effects, yields coefficients involving all factors of interest. This suggests a geometric view, with affine transformations of counts of runs determining partial aliasing properties. Fontana (2013) provides another view on Kronecker products.

140 *Example 1.* Consider the design in Table 2. As this is an orthogonal array of strength 2, nonzero indicator coefficients must involve at least three factors. By counting the $|\mathcal{F}_{123,T_1T_2T_3}|$,

$$\begin{aligned} A_1 \otimes A_2 \otimes A_3 &= 2^{-3} 3^{-1} \left\{ \bigotimes_{j=1}^3 \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \right\} (0, 0, 1, 0, 1, 0, 0, 1)' - \left(0, 0, 0, 0, 0, 0, 0, \frac{1}{9} \right)' \\ &= \left(-\frac{1}{8}, -\frac{1}{24}, \frac{1}{24}, -\frac{1}{24}, \frac{1}{24}, -\frac{1}{24}, \frac{1}{24}, \frac{1}{72} \right)'. \end{aligned}$$

145 Similar computations are performed for $A_1 \otimes A_2 \otimes A_4$, $A_1 \otimes A_3 \otimes A_4$ and $A_2 \otimes A_3 \otimes A_4$, leading to the result that $A_1 \otimes A_2 \otimes A_3 \otimes A_4 = (0, \dots, 0)'$. Thus, two-factor interactions involving distinct factors are orthogonal in this design.

Table 2. Design with $A_3 = A_1 + A_2$, $A_4 = A_1 + 2A_2$ modulo 3. Four columns on the left represent it under field notation, and the four on the right represent it using linear-quadratic notation.

Field Theory				Linear-Quadratic			
A_1	A_2	A_3	A_4	A_1	A_2	A_3	A_4
0	0	0	0	-1	-1	-1	-1
0	1	1	2	-1	0	0	1
0	2	2	1	-1	1	1	0
1	0	1	1	0	-1	0	0
1	1	2	0	0	0	1	-1
1	2	0	2	0	1	-1	1
2	0	2	2	1	-1	1	1
2	1	0	1	1	0	-1	0
2	2	1	0	1	1	0	-1

Example 2. Construction of an $\text{OA}(18, 6, 3, 2)$ by the Kronecker sum operation on a difference matrix (Wang & Wu, 1991) makes calculation of the indicator function particularly enlightening. The difference matrix $D_{6,6;3}$ is defined as

$$D_{6,6;3} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 2 & 1 & 1 & 0 & 2 \\ 0 & 0 & 2 & 1 & 2 & 1 \\ 0 & 2 & 0 & 2 & 1 & 1 \\ 0 & 1 & 1 & 2 & 2 & 0 \end{pmatrix},$$

and the array is constructed by the following transformation involving addition modulo 3:

$$\begin{pmatrix} D_{6,6;3} \\ D_{6,6;3} + J \text{ modulo } 3 \\ D_{6,6;3} + 2J \text{ modulo } 3 \end{pmatrix},$$

150 where J is the 6×6 matrix with all entries equal to 1. The correspondence between runs 7–12 and 1–6, and also between runs 13–18 and 1–6, illuminates the calculation of indicator function coefficients. For example, for distinct factors i_1, i_2, i_3 ,

$$|\mathcal{F}_{i_1 i_2 i_3, \text{LLL}}| = |\mathcal{F}_{i_1 i_2 i_3, \text{QQQ}}| = \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2} = x_{i_3}}} 1 = 1.$$

In addition,

$$|\mathcal{F}_{i_1 i_2 i_3, \text{LLQ}}| = \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}, \\ x_{i_3} = x_{i_1} + 1}} 1, \quad |\mathcal{F}_{i_1 i_2 i_3, \text{QQL}}| = \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}, \\ x_{i_3} = x_{i_1} + 2}} 1.$$

From the definition of a difference matrix,

$$\sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}}} 1 = \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2} = x_{i_3}}} 1 + \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}, \\ x_{i_3} = x_{i_1} + 1}} 1 + \sum_{\substack{x \in D_{6,6;3}: \\ x_{i_1} = x_{i_2}, \\ x_{i_3} = x_{i_1} + 2}} 1 = 2,$$

hence $|\mathcal{F}_{i_1 i_2 i_3, \text{QQL}}| = 1 - |\mathcal{F}_{i_1 i_2 i_3, \text{LLQ}}|$. Similarly, $|\mathcal{F}_{i_1 i_2 i_3, \text{QLQ}}| = 1 - |\mathcal{F}_{i_1 i_2 i_3, \text{LQL}}|$ and $|\mathcal{F}_{i_1 i_2 i_3, \text{QLL}}| = 1 - |\mathcal{F}_{i_1 i_2 i_3, \text{LQQ}}|$. Thus, only $|\mathcal{F}_{i_1 i_2 i_3, \text{LLL}}|$, $|\mathcal{F}_{i_1 i_2 i_3, \text{LLQ}}|$, $|\mathcal{F}_{i_1 i_2 i_3, \text{LQL}}|$, and $|\mathcal{F}_{i_1 i_2 i_3, \text{LQQ}}|$ are necessary to calculate $A_{i_1} \otimes A_{i_2} \otimes A_{i_3}$, and each is 0 or 1, as determined by $D_{6,6;3}$ in the manner described above. 155

These calculations highlight an analogy between the construction of a design and its analysis under the linear-quadratic system, and the construction of regular fractional factorials and their analysis under orthogonal components. Field theory provides both a method to construct designs, namely, regular fractions, and a corresponding method of analysis, the orthogonal components system, that facilitates calculations of aliasing relations. For the linear-quadratic system, calculations for indicator coefficients, hence partial aliasing relations, are built through the \otimes operation in a similar manner for designs constructed by transformations of generators, e.g., orthogonal arrays based on difference matrices. Constructing a design through its rows is important for the linear-quadratic system, and such designs, referred to as generator-transformation designs, are to the linear-quadratic system as regular fractions are to orthogonal components. Cheng & Wu (2001) and Bulutoglu & Cheng (2003) provide further examples of such designs. 160

4. PARTIAL ALIASING RELATIONS FOR $\text{OA}(3^n, s, 3, n)$ 170

Proposition 1 aids in the exploration of partial aliasing relations in $\text{OA}(3^n, s, 3, n)$ by facilitating derivations of relationships among indicator function coefficients. It is used to prove that coefficients for any $n + 1$ factors are invariant to permutation of linear and quadratic effects in absolute value, and that coefficients for any $n + 2$ factors are zero.

PROPOSITION 2. For factors A_1, \dots, A_{n+1} in an $\text{OA}(3^n, s, 3, n)$ and $T_1, \dots, T_{n+1} \in \{\text{L}, \text{Q}\}$, 175

$$|b_{1 \dots (n+1), T_1 \dots T_{n+1}}| = |b_{1 \dots (n+1), T_{\psi(1)} \dots T_{\psi(n+1)}}|$$

for any permutation ψ on $\{1, \dots, n + 1\}$.

COROLLARY 1. For a design with $A_{n+1} = c_0 + c_1 A_1 + \dots + c_n A_n$ modulo 3, where A_1, \dots, A_n form an orthogonal array of strength n and $c_0, \dots, c_n \in \{0, 1, 2\}$,

$$|b_{1 \dots (n+1), T_1 \dots T_{n+1}}| = |b_{1 \dots (n+1), T_{\psi(1)} \dots T_{\psi(n+1)}}|$$

for any $T_1, \dots, T_{n+1} \in \{\text{L}, \text{Q}\}$ and permutation ψ on $\{1, \dots, n + 1\}$. 180

To illustrate, for Table 1, $|b_{123, \text{LLQ}}| = |b_{123, \text{LQL}}| = |b_{123, \text{QLL}}|$ and $|b_{123, \text{LQQ}}| = |b_{123, \text{QLQ}}| = |b_{123, \text{QQL}}|$. If a design had $b_{123, \text{LLQ}} = 0$, with A_1, A_2 , and A_3 forming a defining relation, then all two-factor linear-linear interactions are uncorrelated with a quadratic main effect, or alternatively all two-factor linear-quadratic interactions are uncorrelated with a linear main effect, for

these factors. For each set of $n + 1$ factors in an $\text{OA}(3^n, s, 3, n)$, their coefficients can be partitioned according to the number of linear and quadratic effects, and their estimable interactions correspond to a $b_{I,T}$ equal to zero and permutations of effects in T .

PROPOSITION 3. *In an $\text{OA}(3^n, s, 3, n)$, $A_1 \otimes \cdots \otimes A_{n+2} = (0, \dots, 0)'$.*

COROLLARY 2. *For a design with*

$$A_{n+1} = c_0 + c_1 A_1 + \cdots + c_n A_n \text{ modulo } 3,$$

$$A_{n+2} = d_0 + d_1 A_1 + \cdots + d_n A_n \text{ modulo } 3,$$

where A_1, \dots, A_n form an orthogonal array of strength n , and $c_0, \dots, c_n, d_0, \dots, d_n \in \{0, 1, 2\}$ with $c_1, \dots, c_n, d_1, \dots, d_n \neq 0$,

$$A_1 \otimes \cdots \otimes A_{n+2} = (0, \dots, 0)'.$$

These results show how two-factor interactions can be orthogonal to n -factor interactions. Another interpretation is of main effects being orthogonal to $(n + 1)$ -factor interactions, if they are valid contrasts. Proposition 3 further eliminates the need to calculate indicator function coefficients guaranteed to be zero for certain designs.

5. CONDITIONS FOR ESTIMABLE INTERACTIONS

Conditions that yield estimable interactions are now considered. As before, Proposition 1 is instrumental in proving these results.

PROPOSITION 4. *For factors A_1, A_2, A_3 forming an orthogonal array of strength 2 in \mathcal{F} , $b_{123, T_1 T_2 L} = 0$ for all $T_1, T_2 \in \{L, Q\}$ if and only if $|\mathcal{F}_{123, T_1 T_2 L}| = |\mathcal{F}_{123, T_1 T_2 Q}|$ for all $T_1, T_2 \in \{L, Q\}$, and it is impossible for $b_{123, T_1 T_2 Q} = 0$ for all $T_1, T_2 \in \{L, Q\}$ if $|\mathcal{F}|/9$ is not divisible by 3.*

PROPOSITION 5. *For factors A_1, A_2, A_3 forming an orthogonal array of strength 2 in \mathcal{F} , if*

$$\sum_{\substack{x \in \mathcal{F}: \\ x_1 x_2 = 1}} X_{3,L}(x) = \sum_{\substack{x \in \mathcal{F}: \\ x_1 x_2 = -1}} X_{3,L}(x) = 0,$$

then $b_{123, LLL} = b_{123, QQL} = 0$. Furthermore, if these factors form a defining relation, then $b_{123, QLQ} = b_{123, LQQ} = 0$.

Proposition 4 gives a necessary and sufficient condition for $(A_3)_L$ to be orthogonal to all two-factor interactions $(A_1 A_2)_{T_1 T_2}$, and a necessary condition for $(A_3)_Q$ to be orthogonal to all $(A_1 A_2)_{T_1 T_2}$. Proposition 5 differs from Proposition 4 because it considers a specific structure on the runs that yields uncorrelated main effects and two-factor interactions. It has the following practical implication: for quantitative factors, with -1 and 1 being the smallest and largest levels, respectively, for each, uncorrelated main effects and two-factor interactions are achievable by having symmetry in a subset of runs. This is expressed in field notation in the following corollary.

COROLLARY 3. *For factors A_1, A_2, A_3 with $A_3 = d_1 A_1 + d_2 A_2$ modulo 3 in \mathcal{F} , $b_{123, LLL} = b_{123, QQL} = b_{123, LQQ} = b_{123, QLQ} = 0$ if and only if $d_1 = d_2 = 2$ modulo 3.*

One may need to design an experiment in which the effect hierarchy principle (Wu & Hamada, 2009, p. 172) is violated, e.g., some factors are more important through two-factor interactions.

The following proposition introduces a design construction technique for the linear-quadratic system that can be useful in such situations.

PROPOSITION 6. *If $A_{n+2} = c_0 + c_1A_1 + \cdots + c_nA_n$ modulo 3, and A_1, \dots, A_n, A_{n+1} form an orthogonal array of strength $n + 1$, then $A_1 \otimes \cdots \otimes A_{n+1} \otimes A_{n+2} = (0, \dots, 0)'$.* 220

COROLLARY 4. *If*

$$A_j = c_0 + c_1A_1 + \cdots + c_nA_n \text{ modulo } 3,$$

$$A_{j'} = d_0 + d_1A_1 + \cdots + d_nA_n + d_{n+1}A_{n+1} + \cdots + d_{n+m}A_{n+m} \text{ modulo } 3,$$

where at least one of $d_{n+i} \neq 0$ modulo 3 for $i = 1, \dots, m$, and A_1, \dots, A_{n+m} form an orthogonal array of strength $n + m$, then $A_1 \otimes \cdots \otimes A_n \otimes A_j \otimes A_{j'} = (0, \dots, 0)'$. 225

To illustrate the statistical relevance of these results, consider designing a three-level fractional factorial with four factors and 27 runs, in which interest is on two-factor interactions. For the 3_{IV}^{4-1} design with $A_4 = A_1 + A_2 + A_3$ modulo 3, certain two-factor interactions are fully aliased with other two-factor interactions under orthogonal components, and are only partially aliased under the linear-quadratic system. Now consider the design with aliasing relation $A_4 = 2A_1 + 2A_2$ modulo 3, with A_1, A_2, A_3 forming an orthogonal array of strength 3. From Corollary 3 and Proposition 6, all two-factor interactions involving distinct factors are orthogonal, $(A_4)_L$ is uncorrelated with $(A_1A_2)_{LL}$, $(A_1A_2)_{QQ}$, and $(A_4)_Q$ is uncorrelated with $(A_1A_2)_{LQ}$, $(A_1A_2)_{QL}$. If the main effects of A_4 are not significant, we can entertain two-factor interactions involving distinct factors, and those involving the same factor will only be partially aliased. Proposition 6 and Corollary 4 offer the interesting possibility of high-order factorial effects being legitimate contrasts, while low-order effects are not: for this design, four-factor interactions are valid contrasts, whereas three-factor interactions of A_1, A_2, A_4 are not. 230 235

6. CONCLUDING REMARKS

The operation and results in this paper help in understanding properties of the linear-quadratic system. For example, Cheng & Ye (2004) provide a definition for the generalized wordlength pattern of a design that involves indicator function coefficients. By virtue of Proposition 1, an expression for the generalized wordlength pattern that makes explicit the contribution of low-order coefficients can be derived. As pointed out by a referee, our operation can be applied to qualitative factors as well, and any permutation in the coding of qualitative variables might lead to designs with different geometric characteristics and models (Cheng & Ye, 2004). 240 245

These results can also aid in deriving bounds on the magnitude of indicator function coefficients, hence on correlations among contrasts, because the \otimes operation only requires counts of ± 1 level combinations. Similarly, calculation of bounds for D - and G -efficiencies should be simpler with this operation, and hence one can better explore and understand the eligibility of designs for factor screening and response surface exploration (Cheng & Wu, 2001). 250

Recall that the linear-quadratic system is generated by reparametrizing the levels of quantitative factors using orthogonal polynomials. Accordingly, the results in this paper can be extended to designs with more than three levels per factor by means of orthogonal polynomials.

Examples presented here used standard field constructions for regular designs. As seen in Example 2, partial aliasing calculations are also transparent for generator-transformation designs. The role of a design's construction in its analysis under the linear-quadratic system is an important question that warrants further investigation. 255

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APPENDIX 1

An additional operation for further simplification of proofs

265 For factors A_1, A_2 , define $A_1 \odot A_2 = (b_{12,LL}, b_{12,LQ})'$, $A_1^2 \odot A_2 = (b_{12,QL}, b_{12,QQ})'$. Here, $A_1 \odot A_2$ and $A_1^2 \odot A_2$ divide $A_1 \otimes A_2$ by whether A_1 has a linear or quadratic effect, so that $A_1 \otimes A_2 = (A_1 \odot A_2, A_1^2 \odot A_2)'$. Sequential application of \otimes and \odot is defined in the manner below:

$$\begin{aligned} A_1 \odot (A_2 \otimes A_3) &= (b_{123,LLL}, b_{123,LLQ}, b_{123,LQL}, b_{123,LQQ})', \\ A_1^2 \odot (A_2 \otimes A_3) &= (b_{123,QLL}, b_{123,QLQ}, b_{123,QQQ})'. \end{aligned}$$

This is easily generalized to more factors, and provides another calculation in lieu of \otimes . For example, for factors A_1, A_2, A_3 forming an orthogonal array of strength two:

$$A_1 \odot (A_2 \otimes A_3) = 2^{-3} 3^{3-s} \left\{ \bigotimes_{j=1}^2 \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \right\} \left(\sum_{x \in \mathcal{F}_{23,LL}} X_{1,L}(x), \sum_{x \in \mathcal{F}_{23,LQ}} X_{1,L}(x), \sum_{x \in \mathcal{F}_{23,QL}} X_{1,L}(x), \sum_{x \in \mathcal{F}_{23,QQ}} X_{1,L}(x) \right)', \quad (\text{A1})$$

$$270 \quad A_1^2 \odot (A_2 \otimes A_3) = 2^{-3} 3^{3-s} \left\{ \bigotimes_{j=1}^2 \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \right\} \left(\sum_{x \in \mathcal{F}_{23,LL}} X_{1,L}(x)^2, \sum_{x \in \mathcal{F}_{23,LQ}} X_{1,L}(x)^2, \sum_{x \in \mathcal{F}_{23,QL}} X_{1,L}(x)^2, \sum_{x \in \mathcal{F}_{23,QQ}} X_{1,L}(x)^2 \right)', \quad (\text{A2})$$

$$- (0, 0, 0, b_{\phi, \phi})'.$$

APPENDIX 2

Proofs

Proof of Proposition 1. First consider the proof of (3), with $k > j + 1$. Now

$$\begin{aligned} 275 \quad & \sum_{x \in \mathcal{F}} X_{i_1,L}(x) \cdots X_{i_j,L}(x) X_{i_{j+1},L}(x)^2 X_{i_{j+1},Q}(x) \cdots X_{i_k,L}(x)^2 X_{i_k,Q}(x) = \\ & \sum_{x \in \mathcal{D}} F(x) X_{i_1,L}(x) \cdots X_{i_j,L}(x) X_{i_{j+1},L}(x)^2 X_{i_{j+1},Q}(x) \cdots X_{i_k,L}(x)^2 X_{i_k,Q}(x) = \\ & \sum_{x \in \mathcal{D}} \sum_{I^* \in \mathcal{P}} \sum_{T^* \in \mathcal{T}_{I^*}} b_{I^*, T^*} X_{I^*, T^*}(x) X_{i_1,L}(x) \cdots X_{i_j,L}(x) X_{i_{j+1},L}(x)^2 X_{i_{j+1},Q}(x) \cdots X_{i_k,L}(x)^2 X_{i_k,Q}(x). \end{aligned}$$

Recalling Lemma 1 and noting that $X_{i,L}(x) = 0$ when $X_{i,Q}(x) = -2$, and $X_{i,Q}(x) = 1$ when $X_{i,L}(x) = \pm 1$, the expression above is rewritten as

$$\begin{aligned} 280 \quad & b_{i_1 \dots i_k, T_1 \dots T_k} \sum_{x \in \mathcal{D}} X_{i_1,L}(x)^2 \cdots X_{i_k,L}(x)^2 + b_{i_1 \dots i_j, T_1 \dots T_j} \sum_{x \in \mathcal{D}} X_{i_1,L}(x)^2 \cdots X_{i_k,L}(x)^2 \\ & + \sum_{m=1}^{k-j-1} \sum_{\substack{l_1, \dots, l_m \in \{j+1, \dots, k\}: \\ l_1 < \dots < l_m}} \left\{ b_{i_1 \dots i_j i_{l_1} \dots i_{l_m}, T_1 \dots T_j T_{l_1} \dots T_{l_m}} \sum_{x \in \mathcal{D}} X_{i_1,L}(x)^2 \cdots X_{i_k,L}(x)^2 \right\}. \end{aligned}$$

This expression is simplified by using the fact that $\sum_{x \in \mathcal{D}} X_{i_1,L}(x)^2 \cdots X_{i_k,L}(x)^2 = 2^k 3^{s-k}$. The remainder of the proposition is proved in a similar fashion. \square

LEMMA B1. For an $\text{OA}(9, s, 3, 2)$, $|b_{123,LLQ}| = |b_{123,LQL}| = |b_{123,QLL}|$ and $|b_{123,LQQ}| = |b_{123,QLQ}| = |b_{123,QQ L}|$. 285

Proof. An $\text{OA}(9, 3, 3, 2)$ is a Latin square. Computing $b_{123,LLQ}$, $b_{123,LQL}$, and $b_{123,QLL}$ for each of the 12 Latin squares of order 3, it follows that $|b_{123,LLQ}| = |b_{123,LQL}| = |b_{123,QLL}|$. The other set of relationships are similarly established. Thus the result is true for $\text{OA}(9, 3, 3, 2)$, and because the projection of an $\text{OA}(9, s, 3, 2)$ on any 3 factors is a Latin square, the result holds for any $s > 2$. \square

Proof of Proposition 2. From Lemma B1, this holds for $n = 2$. Assume it is true for $n = m$, where $m \geq 2$. Then consider $m + 2$ factors A_1, \dots, A_{m+2} in an orthogonal array \mathcal{F} of strength $m + 1$ with 3^{m+1} runs. We see that 290

$$\begin{aligned} \sum_{x \in \mathcal{F}} X_{1,L}(x) \cdots X_{m+1,L}(x) X_{m+2,L}(x)^2 &= - \sum_{x \in \mathcal{F}_{1,Q}} X_{2,L}(x) \cdots X_{m+1,L}(x) X_{m+2,L}(x)^2 \\ &\quad + \sum_{x \in \mathcal{F}_{1,L}} X_{2,L}(x) \cdots X_{m+1,L}(x) X_{m+2,L}(x)^2. \end{aligned}$$

As \mathcal{F} is an orthogonal array of strength $m + 1$, for all $x \in \mathcal{F}_{1,Q}$, any m factors chosen from A_2, \dots, A_{m+2} form an orthogonal array of strength m and 3^m runs. The same statement holds true for all $x \in \mathcal{F}_{1,L}$. By the inductive hypothesis, we have 295

$$\begin{aligned} - \sum_{x \in \mathcal{F}_{1,Q}} X_{2,L}(x) \cdots X_{m+1,L}(x) X_{m+2,L}(x)^2 &= \mp \sum_{x \in \mathcal{F}_{1,Q}} X_{2,L}(x) \cdots X_{m+1,L}(x)^2 X_{m+2,L}(x), \\ \sum_{x \in \mathcal{F}_{1,L}} X_{2,L}(x) \cdots X_{m+1,L}(x) X_{m+2,L}(x)^2 &= \pm \sum_{x \in \mathcal{F}_{1,L}} X_{2,L}(x) \cdots X_{m+1,L}(x)^2 X_{m+2,L}(x), \end{aligned}$$

so that

$$\sum_{x \in \mathcal{F}} X_{1,L}(x) \cdots X_{m+1,L}(x) X_{m+2,L}(x)^2 = \pm \sum_{x \in \mathcal{F}} X_{1,L}(x) \cdots X_{m+1,L}(x)^2 X_{m+2,L}(x).$$

From Proposition 1, these equalities establish that $|b_{1\dots(m+2),L\dots LQ}| = |b_{1\dots(m+2),L\dots QL}|$. The other equalities follow similarly, thus completing the induction step. \square 300

LEMMA B2. For factors A_1, A_2, A_3, A_4 in an $\text{OA}(9, s, 3, 2)$, $A_1 \otimes A_2 \otimes A_3 \otimes A_4 = (0, \dots, 0)'$.

Proof. The proof follows in a similar manner as that of Lemma B1 by noting that the projection of the $\text{OA}(9, s, 3, 2)$ on any four factors is a Graeco-Latin square, and applying Proposition 1. \square

Proof of Proposition 3. A similar induction argument as in Proposition 2, combined with Lemma B2 and the relations among the indicator function coefficients given in Proposition 1, yields the result. \square 305

Proof of Proposition 4. The first statement follows from (A1) and the fact that the Hadamard matrix in this equation is non-singular. To prove the second, $A_3^2 \odot (A_1 \otimes A_2)$ in (A2) is written as:

$$2^{-3} 3^{3-s} \left\{ \bigotimes_{j=1}^2 \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \right\} \left\{ \begin{pmatrix} \sum_{x \in \mathcal{F}_{12,LL}} X_{3,L}(x)^2 \\ \sum_{x \in \mathcal{F}_{12,LQ}} X_{3,L}(x)^2 \\ \sum_{x \in \mathcal{F}_{12,QL}} X_{3,L}(x)^2 \\ \sum_{x \in \mathcal{F}_{12,QQ}} X_{3,L}(x)^2 \end{pmatrix} - 2^1 3^{s-3} \begin{pmatrix} \frac{k}{3^{s-2}} \\ \frac{k}{3^{s-2}} \\ \frac{k}{3^{s-2}} \\ \frac{k}{3^{s-2}} \end{pmatrix} \right\},$$

where $k = |\mathcal{F}|/9$. The expression above is $(0, \dots, 0)'$ if and only if

$$\sum_{x \in \mathcal{F}_{12,LL}} X_{3,L}(x)^2 = \sum_{x \in \mathcal{F}_{12,LQ}} X_{3,L}(x)^2 = \sum_{x \in \mathcal{F}_{12,QL}} X_{3,L}(x)^2 = \sum_{x \in \mathcal{F}_{12,QQ}} X_{3,L}(x)^2 = \frac{2k}{3},$$

310 which is impossible if k is not divisible by 3. \square

Proof of Proposition 5. This follows in a straightforward manner from (A1), (A2), and Corollary 1. \square

Proof of Proposition 6. First, note that for $a_1, \dots, a_n, a_{n+2} \in \{1, 2\}$,

$$\begin{aligned} \sum_{x \in \mathcal{F}} X_{1,L}(x)^{a_1} \cdots X_{n,L}(x)^{a_n} X_{n+1,L}(x) X_{n+2,L}(x)^{a_{n+2}} = \\ \sum_{x \in \mathcal{F}_{n+1,L}} X_{1,L}(x)^{a_1} \cdots X_{n,L}(x)^{a_n} X_{n+2,L}(x)^{a_{n+2}} - \sum_{x \in \mathcal{F}_{n+1,Q}} X_{1,L}(x)^{a_1} \cdots X_{n,L}(x)^{a_n} X_{n+2,L}(x)^{a_{n+2}}. \end{aligned}$$

315 As A_1, \dots, A_n, A_{n+1} form an orthogonal array of strength $n+1$, the expression above is zero, and so by Proposition 1, $A_{n+1} \odot (A_1 \otimes \cdots \otimes A_n \otimes A_{n+2}) = (0, \dots, 0)'$. A similar reasoning leads to $A_{n+1}^2 \odot (A_1 \otimes \cdots \otimes A_n \otimes A_{n+2}) = (0, \dots, 0)'$, establishing the proposition. \square

REFERENCES

- BULUTOGLU, D. A. & CHENG, C.-S. (2003). Hidden projection properties of some nonregular fractional factorial designs and their applications. *Annals of Statistics* **31**, 1012–1026.
- 320 CHENG, S. W. & WU, C. F. J. (2001). Factor screening and response surface exploration (with discussion). *Statistica Sinica* **11**, 553–604.
- CHENG, S. W. & YE, K. Q. (2004). Geometric isomorphism and minimum aberration for factorial designs with quantitative factors. *The Annals of Statistics* **32**, 2168–2185.
- 325 FONTANA, R. (2013). Algebraic generation of minimum size orthogonal fractional factorial designs: an approach based on integer linear programming. *Computational Statistics* **28**, 241–253.
- FONTANA, R., PISTONE, G. & ROGANTIN, M. P. (2000). Classification of two-level factorial fractions. *Journal of Statistical Planning and Inference* **87**, 149–172.
- HAMADA, M. S. & WU, C. F. J. (1992). Analysis of designed experiments with complex aliasing. *Journal of Quality Technology* **24**, 130–137.
- 330 PISTONE, G. & ROGANTIN, M. P. (2008). Indicator function and complex coding for mixed fractional factorial designs. *Journal of Statistical Planning and Inference* **133**, 787–802.
- PISTONE, G. & WYNN, H. P. (1996). Generalised confounding with Gröbner bases. *Biometrika* **83**, 653–666.
- WANG, J. C. & WU, C. F. J. (1991). An approach to the construction of asymmetrical orthogonal arrays. *Journal of the American Statistical Association* **86**, 450–456.
- 335 WU, C. F. J. & HAMADA, M. S. (2009). *Experiments: Planning, Analysis, and Optimization*. Wiley Series in Probability and Statistics. Wiley, 2nd ed.
- YE, K. Q. (2003). Indicator function and its application in two-level factorial designs. *The Annals of Statistics* **31**, 984–994.
- 340 YE, K. Q. (2004). A note on regular fractional factorial designs. *Statistica Sinica* **14**, 1069–1074.

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