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CHARACTERIZING AND COMPARING ORDER-OF-ADDITION ORTHOGONAL ARRAYS

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Abstract: Given a set of parameters, several non-isomorphic order-of-addition orthogonal arrays can be generated to design an order-of-addition experiment. Under resource constraints, selecting the best from these candidate designs for the experiment can be practical to extract as much information as possible from the observed data. Based on some theoretical results developed for two-level orthogonal arrays, a series of numerical indices called centralized generalized wordlength pattern is proposed in this paper to characterize and compare order-of-addition orthogonal arrays. Specifically, the J-characteristics are first justified for pairwise order matrices when the transitive property of pairwise order factors is taken into account. The centralized generalized wordlength pattern is then defined based on the sums of squared differences between the normalized J-characteristics of the pairwise order matrices determined by the fractional and full designs. Essentially, it can be viewed as a natural extension of the generalized wordlength pattern used for two-level orthogonal arrays. Their functional relationship is further simplified such that the computational cost can be reduced significantly. Some optimal order-of-addition orthogonal arrays with economical run sizes are identified from existing catalogues for future work.

Key words and phrases: Hadamard matrix; Hamming distance; Inversion; J-characteristic; Projection property.

1 Introduction

Order-of-addition experiments are often conducted to explore optimal addition orders of several components in some agricultural, chemical, industrial and pharmaceutical studies. Some real-world order-of-addition problems were introduced by Voelkel and Gallagher (2019) and Wang, Xu and Ding (2020). Because every component is fixed at a constant level throughout an experiment, the concept of factors used in conventional theory of experimental designs cannot be applied directly when designing an order-of-addition experiment. Therefore, efficient designs for such experiments have received increasing attention from researchers and practitioners in recent years. Van Nostrand (1995) first used a series of pseudo factors taking values ± 1 to denote whether or not a particular component is added before another component. Following this line of thought, Voelkel (2019) proposed order-of-addition orthogonal arrays to design these kinds of experiments, where the pseudo factors were formally called the pairwise order factors. By definition, a pairwise order matrix of entries ± 1 is called an order-of-addition orthogonal array of strength t if, for any t columns, the frequencies of all ordered t-tuples are proportional to those of the pairwise order matrix corresponding to the full design. Because the pairwise order matrix determined by the full design is not column-orthogonal, that is, its column vectors have some non-zero inner products, none of the order-of-addition orthogonal arrays are column-orthogonal, with the result that most conventional methods are not valid to characterize optimal designs for order-of-addition experiments. Based on the theoretical results developed by Peng, Mukerjee and Lin (2019), an order-of-addition design is ϕ-optimal for estimating the overall mean and all main effects of the pairwise order factors if the corresponding pairwise order matrix is an order-of-addition orthogonal array of strength two. Specifically, a ϕ-optimal design achieves the theoretical maximum for every concave and signed permutation invariant optimality criterion. Many alphabetic-optimality criteria with statistically meaningful interpretations, such as the A-, D-, E- and MS-optimality criteria, are included in this important class of optimality criteria. Schoen and Mee (2023) further proved that this order-of-addition design is also D-, G- and I-optimal for estimating the linear component-position model proposed by Stokes and Xu (2022). Based on these optimality results, several combinatorial and computational methods have been developed to generate order-of-addition orthogonal arrays. Recent proposals include those by Chen, Mukerjee and Lin (2020), Tsai (2022), Zhao, Dong and Zhao (2022) and Zhao, Lin and Liu (2022).

In addition to active main effects of the pairwise order factors, as noted in Voelkel and Gallagher (2019), Mee (2020) and Wang and Lin (2023), active interaction effects may also play a vital role in addressing order-of-addition problems. Under the sparsity-of-effects assumption, that is, only few effects have a substantial impact on the responses, a two-stage analysis strategy is frequently applied to explore both kinds of active effects. First, significant main effects are screened out by fitting the main effects model to the observed data. Next, the pairwise order matrix is projected onto those significant pairwise order factors to get a tentative model for testing whether or not their interaction effects are also significant. Based on all identified active effects, a final model can then be built to determine an optimal order. This simple strategy was used by Voelkel and Gallagher (2019), Mee (2020) and Tsai (2023b) to analyze some real-world datasets. Order-of-addition designs based on order-of-addition orthogonal arrays of strength two have been known to be optimal for the first-stage analysis. However, when designing an experiment, it is not known which subset of pairwise order factors will be identified to study their interaction effects. Therefore, an order-of-addition orthogonal array would be preferable if it is able to extract as much information as possible from the observed data for the second-stage analysis. Because the full design contains the most comprehensive information regarding the treatment-response relationship, it can be used as a common reference. Specifically, when comparing two fractional designs, one would be preferred over the other if it is more similar, in some sense, to the full design. This simple concept will be formulated more rigorously in the subsequent sections. Under the hierarchy-of-effects assumption, that is, lower-order effects are more important than higher-order effects and effects of the same order are equally important, several selection criteria, such as the maximum generalized resolution by Deng and Tang (1999), minimum G_2-aberration by Tang and Deng (1999) and minimum moment aberration by Xu (2003), have been proposed to evaluate two-level orthogonal arrays. By definition, a design matrix of entries ± 1 is called a two-level orthogonal array of strength t if, for any t columns, the frequencies of all ordered t-tuples are equal. Although the entries of order-of-addition orthogonal arrays and two-level orthogonal arrays take values ± 1, their combinatorial properties are quite different. A key difference is that the design matrix of the full factorial design is not identical to the pairwise order matrix of the full order-of-addition design, with the result that several existing results developed for two-level orthogonal arrays do not seem to be well-justified for order-of-addition orthogonal arrays. Therefore, a tailored series of numerical indices is required to identify an optimal order-of-addition orthogonal array to design an experiment. This paper aims to address this research question.

The remainder of this paper is organized as follows. Section 2 introduces some fundamentals. A series of numerical indices called centralized generalized wordlength pattern is proposed in Section 3. The relationship between the centralized and non-centralized generalized wordlength patterns is studied. In addition, some optimal order-of-addition orthogonal arrays are identified from existing catalogues for future work. Concluding remarks are given in the final section. All proofs are deferred to Appendix.

2 Notation and Definitions

Some key concepts and technical terminologies are introduced in this section.

2.1 Inversions and Pairwise Order Factors

Given a positive integer m, let t_h denote a permutation of $\{1, 2, \ldots, m\}$ given by $t_h = t_{h,1}t_{h,2}\cdots t_{h,m}$. It can be used as a treatment to study m components in an order-of-addition experiment. To conduct the treatment t_h, a researcher must add these m components sequentially according to the order specified by t_h. The permutation in natural order is represented by $t_1 = 12\cdots m$. Let $\mathcal{T}$ denote the set consisting of all m-element permutations given by $\mathcal{T} = \{t_h : h \in \mathcal{U}\}$, where $\mathcal{U} = \{1, 2, \ldots, N\}$ and $|\mathcal{T}| = |\mathcal{U}| = m! = N$. Note that $|\cdot|$ is used to represent the cardinality of a set. From an experimental design perspective, $\mathcal{T}$ can be viewed as the full design that contains the most comprehensive information regarding the treatment-response relationship. Often, it is impractical to conduct all N permutations in $\mathcal{T}$ when $m > 5$. Let $\mathcal{D}$ denote a subset of $\mathcal{T}$ given by $\mathcal{D} = \{t_h : h \in \mathcal{V}\}$, where $\mathcal{V} \subseteq \mathcal{U}$ and $|\mathcal{D}| = |\mathcal{V}| = n \leq N$. To reduce the cost, $\mathcal{D}$ can be used as a fractional design that has a more economical run size. Naturally, $\mathcal{D}$ contains less information than $\mathcal{T}$. Under resource constraints, however, $\mathcal{D}$ would be considered cost-efficient if it contains the same per-observation information as $\mathcal{T}$ for certain user-specified models.

An ordered pair $(t_{h,u}, t_{h,v})$, where $t_{h,u}$ and $t_{h,v}$ represent the uth and vth elements of t_h, is called an inversion if $u < v$ but $t_{h,u} > t_{h,v}$. The inversion number of t_h, denoted by $inv(t_h)$, is a non-negative integer ranging from 0 to $q = m(m-1)/2$. It is a simple measure of sortedness that is often used to develop sorting algorithms. Bóna (2022) provided a comprehensive introduction to inversions and related permutation statistics. Let $z_{h,ij}$ denote the pairwise order factor given by

$$z_{h,ij} = \begin{cases} +1 & \text{if } (j,i) \text{ is not an inversion of } t_h; \\ -1 & \text{if } (j,i) \text{ is an inversion of } t_h, \end{cases}$$

where i and j are positive integers and $1 \leq i < j \leq m$. Given an m-element permutation t_h, a $q \times 1$ pairwise order vector $z_{h,\mathcal{Q}}$ can be obtained by collecting all pairwise order factors indexed by $\mathcal{Q} = \{ij :$ i and j are positive integers and $1 \leq i < j \leq m\}$, where $|\mathcal{Q}| = q$. Because t_1 has no inversion, one has $z_{1,\mathcal{Q}} = 1_q$, where 1_q denotes the $q \times 1$ vector of ones. Let $Z_{\mathcal{U},\mathcal{Q}}$ represent the $N \times q$ pairwise order matrix corresponding to $\mathcal{T}$. To be specific, $Z_{\mathcal{U},\mathcal{Q}}$ consists of all pairwise order vectors $z_{1,\mathcal{Q}}, z_{2,\mathcal{Q}}, \ldots, z_{N,\mathcal{Q}}$ as row vectors. The $n \times q$ pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$ determined by $\mathcal{D}$ can be obtained by deleting the $N-n$ pairwise order vectors indexed by $\mathcal{U} \setminus \mathcal{V}$ from $Z_{\mathcal{U},\mathcal{Q}}$. Formally, a pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$ is called an order-of-addition orthogonal array of strength t, denoted by OofA-OA(n, m, t), if, for any $n \times t$ submatrix of $Z_{\mathcal{V},\mathcal{Q}}$, the frequencies of all ordered t-tuples are proportional to those of the corresponding $N \times t$ submatrix of $Z_{\mathcal{U},\mathcal{Q}}$. Note that order-of-addition orthogonal arrays are defined based on pairwise order matrices instead of design matrices. Obviously, $Z_{\mathcal{U},\mathcal{Q}}$ is an OofA-OA(N, m, q) and it is unique up to isomorphism. Two pairwise order matrices are said to be isomorphic if one can be obtained from the other by interchanging row vectors and/or relabeling components.

Given the pairwise order matrix $Z_{\mathcal{U},\mathcal{Q}}$, its distance distribution is denoted by $[B_0(\mathcal{U}), B_1(\mathcal{U}), \ldots, B_q(\mathcal{U})]$, where

$$B_k(\mathcal{U}) = \frac{1}{N}|\{(z_{g,\mathcal{Q}}, z_{h,\mathcal{Q}}) : d_H(z_{g,\mathcal{Q}}, z_{h,\mathcal{Q}}) = k \text{ and } g, h \in \mathcal{U}\}|,$$

and $d_H(z_{g,\mathcal{Q}}, z_{h,\mathcal{Q}})$ represents the Hamming distance between $z_{g,\mathcal{Q}}$ and $z_{h,\mathcal{Q}}$, that is, the number of pairwise order factors that differ. Specifically, the Hamming distance between $z_{1,\mathcal{Q}}$ and $z_{h,\mathcal{Q}}$ is equal to the inversion number $inv(t_h)$. Note also that $inv(t_h)$ is equal to the number of negative ones in $z_{h,\mathcal{Q}}$. Let $b(m, k)$ denote the number of all m-element permutations with k inversions given by

$$b(m, k) = |\{t_h : inv(t_h) = k \text{ and } h \in \mathcal{U}\}|.$$

Given a positive integer m, the numbers $[b(m, 0), b(m, 1), \ldots, b(m, q)]$ can be obtained using the following generating function:

$$\begin{aligned} F_m(x) &= \prod_{i=1}^{m}\sum_{j=0}^{i-1} x^j \\ &= (1 + x + x^2 + \cdots + x^{m-1})F_{m-1}(x). \end{aligned}$$

The generating function $F_m(x)$ can be obtained by mathematical induction. A rigorous proof can be found in Theorem 2.3 of Bóna (2022). The number $b(m, k)$ is the coefficient of x^k in $F_m(x)$. Based on the recursive relation between $F_m(x)$ and $F_{m-1}(x)$, the numbers $[b(m, 0), b(m, 1), \ldots, b(m, q)]$ can be generated systematically for various values of m. The integer sequence labeled A008302 on the Online Encyclopedia of Integer Sequences (https://oeis.org) consists of these numbers for m up to 50.

Proposition 1. Given a positive integer m, one has $B_k(\mathcal{U}) = b(m, k)$ for $k = 0, 1 \ldots, q$.

Although the values of $B_k(\mathcal{U})$ and $b(m, k)$ are equal, their computational costs are different. The complexities of computing $[B_0(\mathcal{U}), B_1(\mathcal{U}), \ldots, B_q(\mathcal{U})]$ and $[b(m, 0), b(m, 1), \ldots, b(m, q)]$ are $O(N^2q^2)$ and $O(N)$. Proposition 1 offers a computationally less expensive alternative to get the distance distribution of $Z_{\mathcal{U},\mathcal{Q}}$. Given a pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$, its distance distribution $[B_0(\mathcal{V}), B_1(\mathcal{V}), \ldots, B_q(\mathcal{V})]$ can be defined by replacing $\mathcal{U}$ and N in $B_k(\mathcal{U})$ with $\mathcal{V}$ and n, respectively. The complexity of getting the distance distribution of $Z_{\mathcal{V},\mathcal{Q}}$ is $O(n^2q^2)$.

2.2 J-characteristics

Let $\mathcal{W}$ represent the power set of $\mathcal{Q}$. That is, all subsets of $\mathcal{Q}$, denoted by $\mathcal{W}_1, \mathcal{W}_2, \ldots, \mathcal{W}_{2^q}$, are collected in $\mathcal{W}$. In particular, let $\mathcal{W}_1 = \emptyset$, where $\emptyset$ represents the empty set. Following Tang (2001), the J-characteristic of $Z_{\mathcal{U},\mathcal{Q}}$ corresponding to $\mathcal{W}_d$ is defined as

$$J_{\mathcal{W}_d}(\mathcal{U}) = \sum_{h\in\mathcal{U}} \prod_{ij\in\mathcal{W}_d} z_{h,ij}.$$

Specifically, let $J_{\mathcal{W}_1}(\mathcal{U}) = J_{\emptyset}(\mathcal{U}) = N$. The $2^q \times 1$ vector consisting of all J-characteristics of $Z_{\mathcal{U},\mathcal{Q}}$ is denoted by $J_{\mathcal{U}} = E_{\mathcal{U},\mathcal{W}}^{\top} 1_N$, where $E_{\mathcal{U},\mathcal{W}}$ is the $N \times 2^q$ matrix given by

$$E_{\mathcal{U},\mathcal{W}} = [\ e_{\mathcal{U},1} \quad e_{\mathcal{U},2} \quad \cdots \quad e_{\mathcal{U},2^q}\ ].$$

The dth column vector of $E_{\mathcal{U},\mathcal{W}}$ has the form

$$e_{\mathcal{U},d} = \odot_{ij\in\mathcal{W}_d} z_{\mathcal{U},ij},$$

where $\odot$ represents the entry-wise product, and $z_{\mathcal{U},ij}$ denotes the $N \times 1$ vector consisting of all pairwise order factors of components i and j indexed by $\mathcal{U}$. Define $e_{\mathcal{U},1} = 1_N$, which corresponds to the overall mean. In addition, $e_{\mathcal{U},d}$ corresponds to a main effect when $|\mathcal{W}_d| = 1$ and it corresponds to a $|\mathcal{W}_d|$-way interaction effect when $|\mathcal{W}_d| \geq 2$. Similarly, the J-characteristic of $Z_{\mathcal{V},\mathcal{Q}}$ corresponding to $\mathcal{W}_d$ is defined as

$$J_{\mathcal{W}_d}(\mathcal{V}) = \sum_{h\in\mathcal{V}} \prod_{ij\in\mathcal{W}_d} z_{h,ij}.$$

The $2^q \times 1$ vector consisting of all J-characteristics of $Z_{\mathcal{V},\mathcal{Q}}$ is denoted by $J_{\mathcal{V}} = E_{\mathcal{V},\mathcal{W}}^{\top} 1_n$, where $E_{\mathcal{V},\mathcal{W}}$ is the $n \times 2^q$ matrix obtained by deleting the row vectors indexed by $\mathcal{U} \setminus \mathcal{V}$ from $E_{\mathcal{U},\mathcal{W}}$.

Example 1. Suppose that three components are to be studied in an order-of-addition experiment. All permutations of $\{1, 2, 3\}$ are listed in Table 1.

Table 1: Pairwise order vectors of three-element permutations and their entry-wise products.

h	t_h	$z_{h,12}$	$z_{h,13}$	$z_{h,23}$	$e_{h,1}$	$e_{h,2}$	$e_{h,3}$	$e_{h,4}$	$e_{h,5}$	$e_{h,6}$	$e_{h,7}$	$e_{h,8}$
1	123	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1
2	132	+1	+1	−1	+1	+1	+1	−1	+1	−1	−1	−1
3	213	−1	+1	+1	+1	−1	+1	+1	−1	−1	+1	−1
4	231	−1	−1	+1	+1	−1	−1	+1	+1	−1	−1	+1
5	312	+1	−1	−1	+1	+1	−1	−1	−1	−1	+1	+1
6	321	−1	−1	−1	+1	−1	−1	−1	+1	+1	+1	−1
$J_{\mathcal{W}_d}(\mathcal{V})$					4	0	2	2	2	−2	0	0
$J_{\mathcal{W}_d}(\mathcal{U})$					6	0	0	0	2	−2	2	0

The set $\mathcal{T} = \{t_h : h \in \mathcal{U}\}$ consists of all three-element permutations, where $\mathcal{U} = \{1, 2, \ldots, 6\}$. The pairwise order factors $z_{h,12}$, $z_{h,13}$ and $z_{h,23}$ in Table 1 indicate whether or not the three inversions $(2, 1)$, $(3, 1)$ and $(3, 2)$ appear in t_h, respectively. Their index set is given by $\mathcal{Q} = \{12, 13, 23\}$ and the power set of $\mathcal{Q}$ is denoted by $\mathcal{W} = \{\mathcal{W}_1, \mathcal{W}_2, \ldots, \mathcal{W}_8\}$, where $\mathcal{W}_1 = \emptyset$, $\mathcal{W}_2 = \{12\}$, $\mathcal{W}_3 = \{13\}$, $\mathcal{W}_4 = \{23\}$, $\mathcal{W}_5 = \{12, 13\}$, $\mathcal{W}_6 = \{12, 23\}$, $\mathcal{W}_7 = \{13, 23\}$ and $\mathcal{W}_8 = \{12, 13, 23\}$. Suppose that only four permutations can be conducted due to resource constraints. The first four permutations in Table 1 are chosen to generate a subset of $\mathcal{T}$, denoted by $\mathcal{D} = \{t_h : h \in \mathcal{V}\}$, where $\mathcal{V} = \{1, 2, 3, 4\}$. All J-characteristics of $Z_{\mathcal{V},\mathcal{Q}}$ and $Z_{\mathcal{U},\mathcal{Q}}$ are also listed in Table 1.

Because the column vectors of $E_{\mathcal{U},\mathcal{W}}$ are linearly dependent, some J-characteristics in $J_{\mathcal{U}} = E_{\mathcal{U},\mathcal{W}}^{\top} 1_N$ can be expressed as linear functions of the others. These functions may look different when different basis vectors are used to represent the remaining column vectors. Mee (2020) observed that $z_{h,ij}z_{h,ik} - z_{h,ij}z_{h,jk} + z_{h,ik}z_{h,jk} = 1$ and $z_{h,ij} - z_{h,ik} + z_{h,jk} = z_{h,ij}z_{h,ik}z_{h,jk}$ for $h \in \mathcal{U}$ and $\{i, j, k\} \subseteq \{1, 2, \ldots, m\}$. Based on the two linear equations, one has $e_{h,5} - e_{h,6} + e_{h,7} = e_{h,1}$ and $e_{h,2} - e_{h,3} + e_{h,4} = e_{h,8}$ for every treatment in Table 1 such that the J-characteristics of $Z_{\mathcal{U},\mathcal{Q}}$ have the following relationships:

$$J_{\mathcal{W}_5}(\mathcal{U}) - J_{\mathcal{W}_6}(\mathcal{U}) + J_{\mathcal{W}_7}(\mathcal{U}) = J_{\mathcal{W}_1}(\mathcal{U}), \tag{1}$$

and

$$J_{\mathcal{W}_2}(\mathcal{U}) - J_{\mathcal{W}_3}(\mathcal{U}) + J_{\mathcal{W}_4}(\mathcal{U}) = J_{\mathcal{W}_8}(\mathcal{U}). \tag{2}$$

Obviously, the two linear equations in (1) and (2) still hold when $\mathcal{U}$ is replaced with $\mathcal{V}$. Mee (2020) also noted that the column vectors of $E_{\mathcal{U},\mathcal{W}}$ can be classified into $m-1$ groups, where the column vector $e_{\mathcal{U},1} = 1_N$ is excluded, and the number of independent column vectors in each group corresponds to a rencontres number. The integer sequence labeled A008290 on the Online Encyclopedia of Integer Sequences (https://oeis.org) consists of these rencontres numbers. However, when four or more components are considered, it is not clear how to express a column vector of $E_{\mathcal{U},\mathcal{W}}$ as a linear combination of the basis vectors. Therefore, there is currently no systematic method to express the functional relationships of all J-characteristics for $m > 3$.

3 Main Results

All theoretical and computational results are presented in this section.

3.1 Characterization

Tang (2001) used J-characteristics to characterize design matrices for two-level factorial experiments. Not surprisingly, J-characteristics can also be used to characterize pairwise order matrices for order-of-addition experiments.

Corollary 1. A pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$ is uniquely determined by its J-characteristics in $J_{\mathcal{V}}$.

Basically, Corollary 1 follows from Theorem 1 of Tang (2001). However, when J-characteristics are used to characterize pairwise order matrices, Tang's (2001) formulation needs to be slightly modified to take the transitive property of pairwise order factors into account. The following example is given to illustrate how this can be done.

Example 2. As shown in Example 1, all pairwise order factors indexed by $\mathcal{Q}$ can be used to convert an m-element permutation t_h to a $(+1, -1)$-vector of length q, denoted by $z_{h,\mathcal{Q}}$. However, some $(+1, -1)$-vectors of length q cannot be converted to m-element permutations. For example, when three-element permutations are considered, there are two such invalid pairwise order vectors given by

$$\begin{aligned} z_{7,\mathcal{Q}} &= [\ z_{7,12} \quad z_{7,13} \quad z_{7,23}\ ]^{\top} \\ &= [\ -1 \quad +1 \quad -1\ ]^{\top}, \end{aligned}$$

and

$$\begin{aligned} z_{8,\mathcal{Q}} &= [\ z_{8,12} \quad z_{8,13} \quad z_{8,23}\ ]^\top \\ &= [\ +1 \quad -1 \quad +1\ ]^\top. \end{aligned}$$

The two pairwise order factors $z_{8,12} = +1$ and $z_{8,23} = +1$ indicate that component 1 needs to be added before component 2 and component 2 needs to be added before component 3 such that component 1 must be added before component 3 and the corresponding pairwise order factor must equal $+1$. The $(+1, -1)$-vector $z_{8,\mathcal{Q}}$ is invalid due to the fact that $z_{8,13} = -1$. By similar arguments, $z_{7,\mathcal{Q}}$ is also invalid. Although $z_{7,\mathcal{Q}}$ and $z_{8,\mathcal{Q}}$ violate the transitive property of pairwise order factors, their entry-wise products can still be calculated. All their entry-wise products are presented in Table 2, where the index set of the two invalid pairwise order vectors $z_{7,\mathcal{Q}}$ and $z_{8,\mathcal{Q}}$ is denoted by $\mathcal{I} = \{7, 8\}$, and the power set $\mathcal{W} = \{\mathcal{W}_1, \mathcal{W}_2, \ldots, \mathcal{W}_8\}$ is given in Example 1.

Table 2: Invalid pairwise order vectors of three-element permutations and their entry-wise products.

h	t_h	$z_{h,12}$	$z_{h,13}$	$z_{h,23}$	$e_{h,1}$	$e_{h,2}$	$e_{h,3}$	$e_{h,4}$	$e_{h,5}$	$e_{h,6}$	$e_{h,7}$	$e_{h,8}$
7	N.A.	-1	$+1$	-1	$+1$	-1	$+1$	-1	-1	$+1$	-1	$+1$
8	N.A.	$+1$	-1	$+1$	$+1$	$+1$	-1	$+1$	-1	$+1$	-1	-1

Let n_h denote the number of observations of t_h. By Corollary 1, the numbers of observations $n_1, n_2, \ldots, n_8$ and the J-characteristics $J_{\mathcal{W}_1}(\mathcal{V}), J_{\mathcal{W}_2}(\mathcal{V}), \ldots, J_{\mathcal{W}_8}(\mathcal{V})$ have the following relationship:

$$\begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \\ n_5 \\ n_6 \\ n_7 \\ n_8 \end{bmatrix} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \\ n_5 \\ n_6 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{8} \begin{bmatrix} +1 & +1 & +1 & +1 & +1 & +1 & +1 & +1 \\ +1 & +1 & +1 & -1 & +1 & -1 & -1 & -1 \\ +1 & -1 & +1 & +1 & -1 & -1 & +1 & -1 \\ +1 & -1 & -1 & +1 & +1 & -1 & -1 & +1 \\ +1 & +1 & -1 & -1 & -1 & -1 & +1 & +1 \\ +1 & -1 & -1 & -1 & +1 & +1 & +1 & -1 \\ +1 & -1 & +1 & -1 & -1 & +1 & -1 & +1 \\ +1 & +1 & -1 & +1 & -1 & +1 & -1 & -1 \end{bmatrix} \begin{bmatrix} J_{\mathcal{W}_1}(\mathcal{V}) \\ J_{\mathcal{W}_2}(\mathcal{V}) \\ J_{\mathcal{W}_3}(\mathcal{V}) \\ J_{\mathcal{W}_4}(\mathcal{V}) \\ J_{\mathcal{W}_5}(\mathcal{V}) \\ J_{\mathcal{W}_6}(\mathcal{V}) \\ J_{\mathcal{W}_7}(\mathcal{V}) \\ J_{\mathcal{W}_8}(\mathcal{V}) \end{bmatrix}. \tag{3}$$

The first six row vectors of the right-hand-side matrix in (3) are determined by the entry-wise products in Table 1 and the last two row vectors are determined by the entry-wise products in Table 2. The right-hand-side matrix in (3) is a Hadamard matrix of order eight and it is invertible. Based on the matrix identity in (3), the numbers of observations $n_1, n_2, \ldots, n_8$ are uniquely determined by the J-characteristics $J_{\mathcal{W}_1}(\mathcal{V}), J_{\mathcal{W}_2}(\mathcal{V}), \ldots, J_{\mathcal{W}_8}(\mathcal{V})$. The transitive property of pairwise order factors imposes two sum-to-zero constraints on the J-characteristics in (3). It is not difficult to see that the two sum-to-zero constraints are determined by the two linear equations in (1) and (2). Therefore, n_7 and n_8 in (3) must equal zero due to the fact that $z_{7,\mathcal{Q}}$ and $z_{8,\mathcal{Q}}$ are invalid pairwise order vectors. More general arguments are detailed in Appendix.

Based on Corollary 1, pairwise order matrices determined by different subsets of $\mathcal{T}$ have different J-characteristics. Although J-characteristics are integer-valued indices ranging from $-n$ to $+n$, their values are restricted to certain integers when characterizing order-of-addition orthogonal arrays of strength two.

Proposition 2. Given an OofA-OA$(n, m, 2)$ for $m \geq 4$, denoted by $Z_{\mathcal{V},\mathcal{Q}}$, one has (a) the value of $J_{\mathcal{W}_d}(\mathcal{V})$ must be a multiple of four and (b) the value of $J_{\mathcal{W}_d}(\mathcal{V})$ must be a multiple of eight if n is a multiple of 24.

By conclusion (b) of Proposition 2, the value of $J_{\mathcal{W}_d}(\mathcal{U})$ must be a multiple of eight because $Z_{\mathcal{U},\mathcal{Q}}$ is an OofA-OA(N, m, q) and $N = m!$ is a multiple of 24 for $m \geq 4$. Often, J-characteristics are normalized when comparing pairwise order matrices of different run sizes. A common reference for such comparisons is $Z_{\mathcal{U},\mathcal{Q}}$.

Theorem 1. A pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$ is an OofA-OA(n, m, t) if and only if $J_{\mathcal{W}_d}(\mathcal{V})/n = J_{\mathcal{W}_d}(\mathcal{U})/N$ for every $\mathcal{W}_d$ with $|\mathcal{W}_d| \leq t$.

For two arbitrary effects indexed by $\mathcal{W}_a$ and $\mathcal{W}_b$, where $|(\mathcal{W}_a \cup \mathcal{W}_b) \setminus (\mathcal{W}_a \cap \mathcal{W}_b)| = |\mathcal{W}_d| \leq t$, if $Z_{\mathcal{V},\mathcal{Q}}$ is an OofA-OA(n, m, t), then, after run-size adjustment, the extent of orthogonality when using $Z_{\mathcal{V},\mathcal{Q}}$ would be identical to the extent of orthogonality when using $Z_{\mathcal{U},\mathcal{Q}}$. Therefore, order-of-addition designs based on order-of-addition orthogonal arrays provide the same per-observation information as the full design for the two effects indexed by $\mathcal{W}_a$ and $\mathcal{W}_b$.

Example 3. Two 12-run order-of-addition designs for four components are listed in Table 2 of Voelkel (2019). The pairwise order factors $z_{h,12}$, $z_{h,13}$, $z_{h,14}$, $z_{h,23}$, $z_{h,24}$ and $z_{h,34}$ are used to convert the two order-of-addition designs to two pairwise order matrices, denoted by $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$, where the index set $\mathcal{Q} = \{12, 13, 14, 23, 24, 34\}$. By comparing the normalized J-characteristics of $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$ with the normalized J-characteristics of $Z_{\mathcal{U},\mathcal{Q}}$, one has

$$\frac{1}{12}J_{\mathcal{W}_d}(\mathcal{V}_1) = \frac{1}{12}J_{\mathcal{W}_d}(\mathcal{V}_2) = \frac{1}{24}J_{\mathcal{W}_d}(\mathcal{U}) = 0 \text{ for every } \mathcal{W}_d \text{ has the form } \{ij\},$$

and

$$\frac{1}{12}J_{\mathcal{W}_d}(\mathcal{V}_1) = \frac{1}{12}J_{\mathcal{W}_d}(\mathcal{V}_2) = \frac{1}{24}J_{\mathcal{W}_d}(\mathcal{U}) = \begin{cases} +1/3 & \text{for every } \mathcal{W}_d \text{ has the form } \{ij, il\} \text{ or } \{ij, kj\}; \\ -1/3 & \text{for every } \mathcal{W}_d \text{ has the form } \{ij, jl\}; \\ 0 & \text{for every } \mathcal{W}_d \text{ has the form } \{ij, kl\}, \end{cases}$$

where $i, j, k, l \in \{1, 2, 3, 4\}$. By Theorem 1, $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$ are OofA-OA$(12, 4, 2)$'s.

Given a permutation $t_h = t_{h,1}t_{h,2}\cdots t_{h,m}$, its reverse is denoted by $rev(t_h) = t_{h,m}t_{h,m-1}\cdots t_{h,1}$. An order-of-addition design $\mathcal{D}$ is called a foldover design if its index set $\mathcal{V}$ can be partitioned into two mutually exclusive subsets $\mathcal{H}$ and $\mathcal{G}$ of the same size such that, for every permutation t_h indexed by $\mathcal{H}$, its reverse $t_g = rev(t_h)$ is indexed by $\mathcal{G}$. Because $z_{g,\mathcal{Q}} = -z_{h,\mathcal{Q}}$ for every $t_g = rev(t_h)$, the pairwise order matrix of a foldover design can be expressed as

$$Z_{\mathcal{V},\mathcal{Q}} = \begin{bmatrix} +1 \\ -1 \end{bmatrix} \otimes Z_{\mathcal{H},\mathcal{Q}}, \tag{4}$$

where $\otimes$ represents the Kronecker product, and $Z_{\mathcal{G},\mathcal{Q}} = -Z_{\mathcal{H},\mathcal{Q}}$.

Theorem 2. A pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$ corresponds to a foldover design $\mathcal{D}$ if and only if $J_{\mathcal{W}_d}(\mathcal{V}) = 0$ for every $\mathcal{W}_d$ with odd $|\mathcal{W}_d|$.

Based on Theorem 2, one has $J_{\mathcal{W}_d}(\mathcal{U}) = 0$ for every $\mathcal{W}_d$ with odd $|\mathcal{W}_d|$ due to the fact that $\mathcal{T}$ is a foldover design.

3.2 Comparison

Although pairwise order matrices are uniquely determined by their J-characteristics, it is impractical to use all J-characteristics to compare pairwise order matrices. Below, a series of summary statistics of J-characteristics is proposed to simplify the comparison procedure.

Definition 1. Given a pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$, the vector $[C_1(\mathcal{V}), C_2(\mathcal{V}), \ldots, C_q(\mathcal{V})]$ is called the centralized generalized wordlength pattern, where

$$C_a(\mathcal{V}) = \sum_{|\mathcal{W}_d|=a} \left[\frac{1}{n} J_{\mathcal{W}_d}(\mathcal{V}) - \frac{1}{N} J_{\mathcal{W}_d}(\mathcal{U})\right]^2 \tag{5}$$

for $a = 1, 2, \ldots, q$.

By Corollary 3 of Tang (2001), the projection properties of $Z_{\mathcal{V},\mathcal{Q}}$ and $Z_{\mathcal{U},\mathcal{Q}}$ onto t pairwise order factors are completely determined by $J_{\mathcal{W}_d}(\mathcal{V})$ and $J_{\mathcal{W}_d}(\mathcal{U})$ with $|\mathcal{W}_d| \leq t$. It can also be seen from Definition 1 that small values of the first t entries of the centralized generalized wordlength pattern reflect the fact that the differences between the corresponding normalized J-characteristics are also small. Therefore, the centralized generalized wordlength pattern can be viewed as a series of similarity measures between $Z_{\mathcal{V},\mathcal{Q}}$ and $Z_{\mathcal{U},\mathcal{Q}}$ when projecting onto various numbers of pairwise order factors. Theorem 1 is now rephrased in terms of the centralized generalized wordlength pattern.

Corollary 2. A pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$ is an OofA-OA(n, m, t) if and only if $C_a(\mathcal{V}) = 0$ for $a \leq t$.

Suppose that two OofA-OA(n, m, t)'s, denoted by $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$, are being evaluated. By Corollary 2, one has $C_a(\mathcal{V}_1) = C_a(\mathcal{V}_2) = 0$ for $a \leq t$. If $C_{t+1}(\mathcal{V}_1) < C_{t+1}(\mathcal{V}_2)$, then $Z_{\mathcal{V}_1,\mathcal{Q}}$ would be considered superior to $Z_{\mathcal{V}_2,\mathcal{Q}}$ because $Z_{\mathcal{V}_1,\mathcal{Q}}$ is more similar to an OofA-OA$(n, m, t+1)$ when projecting onto $t+1$ pairwise order factors. However, if $C_{t+1}(\mathcal{V}_1) = C_{t+1}(\mathcal{V}_2)$, then the one with a smaller value of $C_{t+2}(\mathcal{V}_i)$ would be preferable. Otherwise, the comparison procedure continues until they can be distinguished by sequentially comparing the values of $C_{t+3}(\mathcal{V}_i), C_{t+4}(\mathcal{V}_i), \ldots, C_q(\mathcal{V}_i)$. By definition, if $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$ are isomorphic, there exists a matrix pair (R, C_1) such that

$$Z_{\mathcal{V}_1,\mathcal{Q}} = R Z_{\mathcal{V}_2,\mathcal{Q}} C_1,$$

where R is a row permutation matrix, and C_1 is a column permutation matrix. Because the column vectors of $E_{\mathcal{V}_1,\mathcal{W}}$ and $E_{\mathcal{V}_2,\mathcal{W}}$ are obtained by entry-wise products of the column vectors of $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$, one has

$$E_{\mathcal{V}_1,\mathcal{W}} = R E_{\mathcal{V}_2,\mathcal{W}} C_2,$$

where C_2 is another column permutation matrix. Note also that two column vectors of $E_{\mathcal{V}_2,\mathcal{W}}$, denoted by $e_{\mathcal{V}_2,a}$ and $e_{\mathcal{V}_2,b}$, is allowed by C_2 to be switched when $|\mathcal{W}_a| = |\mathcal{W}_b|$. Because $R^\top 1_n = 1_n$, one has

$$\begin{aligned} J_{\mathcal{V}_1} &= E_{\mathcal{V}_1,\mathcal{W}}^\top 1_n \\ &= C_2^\top E_{\mathcal{V}_2,\mathcal{W}}^\top R^\top 1_n \\ &= C_2^\top E_{\mathcal{V}_2,\mathcal{W}}^\top 1_n \\ &= C_2^\top J_{\mathcal{V}_2}. \end{aligned}$$

Therefore, $J_{\mathcal{V}_1}$ can be obtained by interchanging the entries of $J_{\mathcal{V}_2}$, with the result that the centralized generalized wordlength patterns of $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$ are identical. Given two non-isomorphic pairwise order matrices, their centralized generalized wordlength patterns may sometimes be identical. A secondary criterion, such as average estimation efficiency over some plausible models, can be used to discriminate between two such pairwise order matrices.

Example 4. Based on Theorem 1, the two pairwise order matrices $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$ in Example 3 are found to be OofA-OA$(12, 4, 2)$'s. Their centralized generalized wordlength patterns are given in Table 3 for further evaluation.

Table 3: Centralized generalized wordlength patterns of two non-isomorphic OofA-OA$(12, 4, 2)$'s.

	$C_1(\mathcal{V}_i)$	$C_2(\mathcal{V}_i)$	$C_3(\mathcal{V}_i)$	$C_4(\mathcal{V}_i)$	$C_5(\mathcal{V}_i)$	$C_6(\mathcal{V}_i)$
$Z_{\mathcal{V}_1,\mathcal{Q}}$	0.000	0.000	1.333	0.000	1.333	0.000
$Z_{\mathcal{V}_2,\mathcal{Q}}$	0.000	0.000	2.222	0.000	0.444	0.000

By Corollary 2, because $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$ are OofA-OA$(12, 4, 2)$'s, one has $C_1(\mathcal{V}_1) = C_1(\mathcal{V}_2) = 0$ and $C_2(\mathcal{V}_1) = C_2(\mathcal{V}_2) = 0$ in Table 3. It can also be seen from Table 3 that $C_3(\mathcal{V}_1) < C_3(\mathcal{V}_2)$. Based on the centralized generalized wordlength pattern, $Z_{\mathcal{V}_1,\mathcal{Q}}$ is considered superior to $Z_{\mathcal{V}_2,\mathcal{Q}}$. Based on different selection criteria, $Z_{\mathcal{V}_1,\mathcal{Q}}$ was also recommended by other researchers. By evaluating the χ^2 measure proposed by Yamada and Lin (1999) and the third power moment proposed by Xu (2003), $Z_{\mathcal{V}_1,\mathcal{Q}}$ was recommended by Voelkel (2019) because of its superior projection properties. In addition, Tsai (2023a) also noted that $Z_{\mathcal{V}_1,\mathcal{Q}}$ is eligible to test all pairwise order dispersion effects. Based on the comparison results, $Z_{\mathcal{V}_1,\mathcal{Q}}$ is recommended for real-world studies.

Example 5. Zhao, Dong and Zhao (2022) listed ten non-isomorphic OofA-OA$(48, 5, 3)$'s in Table A2 of their paper. Their centralized generalized wordlength patterns are given in Table 4 for further discrimination.

Table 4: Centralized generalized wordlength patterns of ten non-isomorphic OofA-OA$(48, 5, 3)$'s.

	$C_1(\mathcal{V}_i)$	$C_2(\mathcal{V}_i)$	$C_3(\mathcal{V}_i)$	$C_4(\mathcal{V}_i)$	$C_5(\mathcal{V}_i)$	$C_6(\mathcal{V}_i)$	$C_7(\mathcal{V}_i)$	$C_8(\mathcal{V}_i)$	$C_9(\mathcal{V}_i)$	$C_{10}(\mathcal{V}_i)$
$Z_{\mathcal{V}_1,\mathcal{Q}}$	0.000	0.000	0.000	3.244	0.000	6.400	0.000	3.156	0.000	0.000
$Z_{\mathcal{V}_2,\mathcal{Q}}$	0.000	0.000	0.000	3.244	0.000	6.844	0.000	2.711	0.000	0.000
$Z_{\mathcal{V}_3,\mathcal{Q}}$	0.000	0.000	0.000	3.689	0.000	6.844	0.000	2.267	0.000	0.000
$Z_{\mathcal{V}_4,\mathcal{Q}}$	0.000	0.000	0.000	3.689	0.000	6.844	0.000	2.267	0.000	0.000
$Z_{\mathcal{V}_5,\mathcal{Q}}$	0.000	0.000	0.000	3.911	0.000	6.844	0.000	2.044	0.000	0.000
$Z_{\mathcal{V}_6,\mathcal{Q}}$	0.000	0.000	0.000	3.467	0.000	7.289	0.000	2.044	0.000	0.000
$Z_{\mathcal{V}_7,\mathcal{Q}}$	0.000	0.000	0.000	3.467	0.000	7.289	0.000	2.044	0.000	0.000
$Z_{\mathcal{V}_8,\mathcal{Q}}$	0.000	0.000	0.000	3.467	0.000	6.844	0.000	2.489	0.000	0.000
$Z_{\mathcal{V}_9,\mathcal{Q}}$	0.000	0.000	0.000	3.022	0.000	7.733	0.000	2.044	0.000	0.000
$Z_{\mathcal{V}_{10},\mathcal{Q}}$	0.000	0.000	0.000	3.689	0.000	7.289	0.000	1.822	0.000	0.000

Based on Corollary 2, because $Z_{\mathcal{V}_1,\mathcal{Q}}, Z_{\mathcal{V}_2,\mathcal{Q}}, \ldots, Z_{\mathcal{V}_{10},\mathcal{Q}}$ are OofA-OA$(48, 5, 3)$'s, the first three entries of all centralized generalized wordlength patterns in Table 4 are equal to zero. By further comparing $C_4(\mathcal{V}_1), C_4(\mathcal{V}_2), \ldots, C_4(\mathcal{V}_{10})$, $Z_{\mathcal{V}_9,\mathcal{Q}}$ is recommended for real-world studies. Most interestingly, it can also be seen that $C_1(\mathcal{V}_i) = C_3(\mathcal{V}_i) = C_5(\mathcal{V}_i) = C_7(\mathcal{V}_i) = C_9(\mathcal{V}_i) = 0$ for $i = 1, 2, \ldots, 10$. By Theorem 2, the ten OofA-OA$(48, 5, 3)$'s in Table 4 correspond to ten foldover designs.

Corollary 3. The pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$ of a foldover design $\mathcal{D}$ in (4) is an OofA-OA$(2n, m, t+1)$ if its submatrix $Z_{\mathcal{H},\mathcal{Q}}$ is an OofA-OA(n, m, t) and t is even.

Based on Proposition 2.3 of Seiden and Zemach (1966), the foldover technique has been commonly used to generate two-level orthogonal arrays of strength three. By Corollary 3, it can also be applied to generate a new order-of-addition orthogonal array of strength three by folding over an existing order-of-addition orthogonal array of strength two.

3.3 Connection

Given a pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$, its generalized wordlength pattern is given by $[A_1(\mathcal{V}), A_2(\mathcal{V}), \ldots, A_q(\mathcal{V})]$, where

$$A_a(\mathcal{V}) = \sum_{|\mathcal{W}_d|=a} \left[\frac{1}{n} J_{\mathcal{W}_d}(\mathcal{V})\right]^2 \tag{6}$$

for $a = 1, 2, \ldots, q$. The minimum G_2-aberration criterion proposed by Tang and Deng (1999) is that it sequentially minimizes the entries of $[A_1(\mathcal{V}), A_2(\mathcal{V}), \ldots, A_q(\mathcal{V})]$. Given a two-level orthogonal array, its centralized generalized wordlength pattern in (5) is equal to its generalized wordlength pattern in (6) because all J-characteristics of the two-level orthogonal array of full strength are equal to zero, except the one corresponding to the empty set $\emptyset$. From this perspective, the centralized generalized wordlength pattern can be viewed as a natural extension of the generalized wordlength pattern because some J-characteristics of $Z_{\mathcal{U},\mathcal{Q}}$ are not equal to zero. In particular, the generalized wordlength pattern of $Z_{\mathcal{U},\mathcal{Q}}$ is given by $[A_1(\mathcal{U}), A_2(\mathcal{U}), \ldots, A_q(\mathcal{U})]$, where

$$A_a(\mathcal{U}) = \sum_{|\mathcal{W}_d|=a} \left[\frac{1}{N} J_{\mathcal{W}_d}(\mathcal{U})\right]^2$$

for $a = 1, 2, \ldots, q$. Based on Theorem 2, because $\mathcal{T}$ is a foldover design, one has $J_{\mathcal{W}_d}(\mathcal{U}) = 0$ for every $\mathcal{W}_d$ with odd $|\mathcal{W}_d|$ such that $A_a(\mathcal{U}) = 0$ for every odd a.

Theorem 3. Given a pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$, one has (a) $C_a(\mathcal{V}) = A_a(\mathcal{V})$ for every odd a and $C_a(\mathcal{V}) = A_a(\mathcal{V}) - A_a(\mathcal{U})$ for every even a, and (b) the sum of the entries of $[C_1(\mathcal{V}), C_2(\mathcal{V}), \ldots, C_q(\mathcal{V})]$ is equal to

$$\sum_{a=1}^{q} C_a(\mathcal{V}) = 2^q \left(\frac{1}{n^2} \sum_{h=1}^{N} n_h^2 - \frac{1}{N}\right),$$

where n_h denotes the number of observations of t_h.

By conclusion (a) of Theorem 3, the centralized generalized wordlength pattern of $Z_{\mathcal{V},\mathcal{Q}}$ is equal to the difference between the generalized wordlength patterns of $Z_{\mathcal{V},\mathcal{Q}}$ and $Z_{\mathcal{U},\mathcal{Q}}$. Because $A_a(\mathcal{U})$ is a fixed constant for every a, ranking results according to the centralized generalized wordlength patterns are consistent with those according to the generalized wordlength patterns. Cheng, Deng and Tang (2002) noted that the generalized wordlength pattern is a good surrogate of some model-dependent optimality criteria to select highly efficient designs for estimating all main effects and some two-factor interaction effects. Based on Theorem 3, their conclusion can also be used to support the centralized generalized wordlength pattern, that is, it tends to yield highly efficient designs for the second-stage analysis. Because $C_a(\mathcal{V})$ is non-negative, one has $A_a(\mathcal{V}) \geq 0$ for every odd a and $A_a(\mathcal{V}) \geq A_a(\mathcal{U})$ for every even a. In other words, $A_a(\mathcal{U})$ is a sharp lower bound of $A_a(\mathcal{V})$ for every a. Theorem 1 is now rephrased in terms of the generalized wordlength pattern.

Corollary 4. A pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$ is an OofA-OA(n, m, t) if and only if $A_a(\mathcal{V}) = 0$ for every odd $a \leq t$ and $A_a(\mathcal{V}) = A_a(\mathcal{U})$ for every even $a \leq t$.

Example 6. The generalized wordlength patterns of the two OofA-OA$(12, 4, 2)$'s in Example 3, denoted by $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$, are given in Table 5. In addition, the generalized wordlength pattern of $Z_{\mathcal{U},\mathcal{Q}}$ is also provided as a reference.

Table 5: Generalized wordlength patterns of two non-isomorphic OofA-OA$(12, 4, 2)$'s.

	$A_1(\mathcal{V}_i)$	$A_2(\mathcal{V}_i)$	$A_3(\mathcal{V}_i)$	$A_4(\mathcal{V}_i)$	$A_5(\mathcal{V}_i)$	$A_6(\mathcal{V}_i)$
$Z_{\mathcal{V}_1,\mathcal{Q}}$	0.000	1.333	1.333	0.333	1.333	0.000
$Z_{\mathcal{V}_2,\mathcal{Q}}$	0.000	1.333	2.222	0.333	0.444	0.000
	$A_1(\mathcal{U})$	$A_2(\mathcal{U})$	$A_3(\mathcal{U})$	$A_4(\mathcal{U})$	$A_5(\mathcal{U})$	$A_6(\mathcal{U})$
$Z_{\mathcal{U},\mathcal{Q}}$	0.000	1.333	0.000	0.333	0.000	0.000

Because $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$ are OofA-OA$(12, 4, 2)$'s, as shown in Table 5, one has $A_1(\mathcal{V}_1) = A_1(\mathcal{V}_2) = A_1(\mathcal{U})$ and $A_2(\mathcal{V}_1) = A_2(\mathcal{V}_2) = A_2(\mathcal{U})$. Based on the minimum G_2-aberration criterion, $Z_{\mathcal{V}_1,\mathcal{Q}}$ is also considered superior to $Z_{\mathcal{V}_2,\mathcal{Q}}$ due to the fact that $A_3(\mathcal{V}_1) < A_3(\mathcal{V}_2)$. This ranking result is consistent with the ranking result in Example 4. It can also be seen from Tables 3 and 5 that $C_a(\mathcal{V}_1) = A_a(\mathcal{V}_1)$ and $C_a(\mathcal{V}_2) = A_a(\mathcal{V}_2)$ for $a = 1, 3, 5$ and $C_a(\mathcal{V}_1) = A_a(\mathcal{V}_1) - A_a(\mathcal{U})$ and $C_a(\mathcal{V}_2) = A_a(\mathcal{V}_2) - A_a(\mathcal{U})$ for $a = 2, 4, 6$.

Because the complexities of computing all J-characteristics in $J_{\mathcal{V}}$ and $J_{\mathcal{U}}$ are $O(n2^q)$ and $O(N2^q)$, it is computationally expensive to get the centralized generalized wordlength pattern using $C_a(\mathcal{V})$ in (5). Ma and Fang (2001) and Xu and Wu (2001) showed that

$$A_a(\mathcal{V}) = \frac{1}{n} \sum_{k=0}^{q} B_k(\mathcal{V}) P_a(k, q, 2),$$

where $P_a(k, q, 2) = \sum_{j=1}^{a} (-1)^j \binom{k}{j} \binom{q-k}{a-j}$ denotes the ath Krawtchouk polynomial. Based on this important result, the generalized wordlength pattern $[A_1(\mathcal{V}), A_2(\mathcal{V}), \ldots, A_q(\mathcal{V})]$ can be computed more quickly because the computational cost of the distance distribution $[B_0(\mathcal{V}), B_1(\mathcal{V}), \ldots, B_q(\mathcal{V})]$ is lower. By Proposition 1, one has

$$\begin{aligned} A_a(\mathcal{U}) &= \frac{1}{N} \sum_{k=0}^{q} B_k(\mathcal{U}) P_a(k, q, 2) \\ &= \frac{1}{N} \sum_{k=0}^{q} b(m, k) P_a(k, q, 2). \end{aligned}$$

The numbers $[b(m,0), b(m,1), \dots, b(m,q)]$ can be obtained systematically using the generating function $F_m(x)$ to speed up the computation of $[A_1(\mathcal{U}), A_2(\mathcal{U}), \dots, A_q(\mathcal{U})]$. Some values of $A_a(\mathcal{U})$ for $4 \le m \le 15$ are collected in the supplementary materials. Based on Theorem 3, one has

$$C_a(\mathcal{V}) = \sum_{k=0}^{q} \left[\frac{1}{n} B_k(\mathcal{V})\right] P_a(k,q,2) \tag{7}$$

for every odd a and

$$C_a(\mathcal{V}) = \sum_{k=0}^{q} \left[\frac{1}{n} B_k(\mathcal{V}) - \frac{1}{N} b(m,k)\right] P_a(k,q,2) \tag{8}$$

for every even a. The centralized generalized wordlength pattern can be computed more quickly using (7) and (8) because the complexities of computing $[B_0(\mathcal{V}), B_1(\mathcal{V}), \dots, B_q(\mathcal{V})]$ and $[b(m,0), b(m,1), \dots, b(m,q)]$ are $O(n^2q^2)$ and $O(N)$.

Example 7. Following Wang and Mee (2022), an OofA-OA$(48, 9, 2)$, denoted by $Z_{\mathcal{V},\mathcal{Q}}$, is generated by adding the pairwise order factors involving the 9th component $z_{h,19}, z_{h,29}, \dots, z_{h,89}$ to every row vector of the OofA-OA$(48, 8, 2)$ provided by Tsai (2022). Based on the D-optimality criterion, a greedy local search procedure is implemented to determine the levels of all additional pairwise order factors. Equivalently, this step can be done by randomly inserting component 9 into every row vector of the design matrix corresponding to the OofA-OA$(48, 8, 2)$. Because $362,880 \times 2^{36}$ entry-wise products must be calculated to get all J-characteristics of $Z_{\mathcal{U},\mathcal{Q}}$, it is time-consuming to compute the centralized generalized wordlength pattern of $Z_{\mathcal{V},\mathcal{Q}}$ using (5). Therefore, it is computed using (7) and (8), where the first six entries are listed in Table 6. In addition, the first six entries of the generalized wordlength patterns of $Z_{\mathcal{V},\mathcal{Q}}$ and $Z_{\mathcal{U},\mathcal{Q}}$ are also provided.

Table 6: Centralized and non-centralized generalized wordlength patterns of an OofA-OA$(48, 9, 2)$.

$C_1(\mathcal{V})$	$C_2(\mathcal{V})$	$C_3(\mathcal{V})$	$C_4(\mathcal{V})$	$C_5(\mathcal{V})$	$C_6(\mathcal{V})$
0.000	0.000	127.778	962.133	7606.222	38555.509
$A_1(\mathcal{V})$	$A_2(\mathcal{V})$	$A_3(\mathcal{V})$	$A_4(\mathcal{V})$	$A_5(\mathcal{V})$	$A_6(\mathcal{V})$
0.000	28.000	127.778	1290.667	7606.222	40686.222
$A_1(\mathcal{U})$	$A_2(\mathcal{U})$	$A_3(\mathcal{U})$	$A_4(\mathcal{U})$	$A_5(\mathcal{U})$	$A_6(\mathcal{U})$
0.000	28.000	0.000	328.533	0.000	2130.713

Because $Z_{\mathcal{V},\mathcal{Q}}$ is an OofA-OA$(48, 9, 2)$, one has $C_1(\mathcal{V}) = C_2(\mathcal{V}) = 0$. It can also be seen from Table 6 that $C_a(\mathcal{V}) = A_a(\mathcal{V})$ for $a = 1, 3, 5$ and $C_a(\mathcal{V}) = A_a(\mathcal{V}) - A_a(\mathcal{U})$ for $a = 2, 4, 6$. As far as I know, this is the first time in the literature that an OofA-OA$(48, 9, 2)$ is obtained. Its design matrix is given in the supplementary materials for future work.

Actually, the centralized and non-centralized generalized wordlength patterns can be used to characterize and compare general pairwise order matrices, even when they are not order-of-addition orthogonal arrays. The following example is given to illustrate how this can be done.

Example 8. Wang and Mee (2022) provided a 12-treatment bias-free design for four components in Table A.2 of their paper. The corresponding pairwise order matrix is denoted by $Z_{\mathcal{V}_3,\mathcal{Q}}$. Because the parameters of $Z_{\mathcal{V}_1,\mathcal{Q}}$ and $Z_{\mathcal{V}_2,\mathcal{Q}}$ in Example 3 and $Z_{\mathcal{V}_3,\mathcal{Q}}$ are identical, their centralized and non-centralized generalized wordlength patterns are given in Table 7 for comparison purposes.

Table 7: Centralized and non-centralized generalized wordlength patterns of $Z_{\mathcal{V}_1,\mathcal{Q}}$, $Z_{\mathcal{V}_2,\mathcal{Q}}$ and $Z_{\mathcal{V}_3,\mathcal{Q}}$.

	$C_1(\mathcal{V}_i)$	$C_2(\mathcal{V}_i)$	$C_3(\mathcal{V}_i)$	$C_4(\mathcal{V}_i)$	$C_5(\mathcal{V}_i)$	$C_6(\mathcal{V}_i)$
$Z_{\mathcal{V}_1,\mathcal{Q}}$	0.000	0.000	1.333	0.000	1.333	0.000
$Z_{\mathcal{V}_2,\mathcal{Q}}$	0.000	0.000	2.222	0.000	0.444	0.000
$Z_{\mathcal{V}_3,\mathcal{Q}}$	0.000	0.333	0.000	1.333	0.000	1.000
	$A_1(\mathcal{V}_i)$	$A_2(\mathcal{V}_i)$	$A_3(\mathcal{V}_i)$	$A_4(\mathcal{V}_i)$	$A_5(\mathcal{V}_i)$	$A_6(\mathcal{V}_i)$
$Z_{\mathcal{V}_1,\mathcal{Q}}$	0.000	1.333	1.333	0.333	1.333	0.000
$Z_{\mathcal{V}_2,\mathcal{Q}}$	0.000	1.333	2.222	0.333	0.444	0.000
$Z_{\mathcal{V}_3,\mathcal{Q}}$	0.000	1.667	0.000	1.667	0.000	1.000

By comparing the first two entries of the centralized and non-centralized generalized wordlength patterns in Table 7, one has $C_2(\mathcal{V}_1) = C_2(\mathcal{V}_2) = 0.000 < 0.333 = C_2(\mathcal{V}_3)$ and $A_2(\mathcal{V}_1) = A_2(\mathcal{V}_2) = 1.333 < 1.667 = A_2(\mathcal{V}_3)$. Based on Corollaries 2 and 4, $Z_{\mathcal{V}_3,\mathcal{Q}}$ is not an OofA-OA$(12, 4, 2)$. However, because $C_1(\mathcal{V}_3) = A_1(\mathcal{V}_3) = 0$ and $C_3(\mathcal{V}_3) = A_3(\mathcal{V}_3) = 0$, one has $J_{\mathcal{W}_d}(\mathcal{V}_3) = 0$ for $|\mathcal{W}_d| = 1$ or $|\mathcal{W}_d| = 3$. Therefore, when the main effects model of the pairwise order factors is used to fit the observed data, the corresponding bias matrix, denoted by

$$(Z_{\mathcal{V}_3,\mathcal{Q}}^\top Z_{\mathcal{V}_3,\mathcal{Q}})^{-1} Z_{\mathcal{V}_3,\mathcal{Q}}^\top E_{\mathcal{V}_3,\mathcal{S}_2},$$

is a zero matrix, where $E_{\mathcal{V}_3,\mathcal{S}_2}$ denotes the 12×15 submatrix of $E_{\mathcal{V}_3,\mathcal{W}}$ consisting of all column vectors indexed by $\mathcal{S}_2 = \{\mathcal{W}_d : |\mathcal{W}_d| = 2\}$. Although $Z_{\mathcal{V}_3,\mathcal{Q}}$ is less efficient in estimating the main effects of the pairwise order factors, as noted in Wang and Mee (2022), it is robust to non-negligible two-factor interaction effects.

Because the two numbers $+1$ and -1 occur equally often in every column vector of $Z_{\mathcal{U},\mathcal{Q}}$, one has $A_1(\mathcal{U}) = 0$. Actually, the values of $A_2(\mathcal{U})$ and $A_q(\mathcal{U})$ also have closed-form expressions.

Proposition 3. Given the pairwise order matrix $Z_{\mathcal{U},\mathcal{Q}}$ for $m \geq 3$, one has (a) $A_2(\mathcal{U}) = m(m-1)(m-2)/18$ and (b) $A_q(\mathcal{U}) = 0$.

By Theorem 4 of Zhao, Lin and Liu (2022), an order-of-addition design is D-optimal for estimating the main effects model of the pairwise order factors if and only if its pairwise order matrix is an order-of-addition orthogonal array of strength two. Based on Corollary 2, Corollary 4 and Proposition 3, their conclusion can be rephrased as follows: an order-of-addition design $\mathcal{D} = \{t_h : h \in \mathcal{V}\}$ is D-optimal if and only if $C_1(\mathcal{V}) = 0$ and $C_2(\mathcal{V}) = 0$, or equivalently, $A_1(\mathcal{V}) = 0$ and $A_2(\mathcal{V}) = m(m-1)(m-2)/18$. Therefore, conclusion (a) of Proposition 3 can be used to get an order-of-addition orthogonal array of strength two by searching for a pairwise order matrix having $A_1(\mathcal{V}) = 0$ and $A_2(\mathcal{V}) = m(m-1)(m-2)/18$. This determinant-free approach is computationally less expensive. By Corollary 4, $A_q(\mathcal{U})$ is equal to zero if q is odd. By conclusion (b) of Proposition 3, it is still equal to zero if q is even.

3.4 Application

All non-isomorphic OofA-OA$(12, 4, 2)$'s and OofA-OA$(12, 5, 2)$'s were obtained by Voelkel (2019) and Zhao, Lin and Liu (2022), respectively. Schoen and Mee (2023) enumerated all non-isomorphic OofA-OA$(24, m, 2)$ for $4 \le m \le 7$. The centralized generalized wordlength pattern is used to rank-order these candidate designs. The identity numbers of optimal order-of-addition orthogonal arrays are listed in Table 8. Below, some interesting observations from these ranking results are summarized. First, the optimal OofA-OA$(24, 4, 6)$ in Table 8 is actually $Z_{\mathcal{U},\mathcal{Q}}$. Second, the centralized generalized wordlength patterns of the two non-isomorphic OofA-OA$(12, 5, 2)$ provided by Zhao, Lin and Liu (2022) are identical. Only the first one is shown in Table 8. Third, because an OofA-OA$(n, m, 3)$ must be an OofA-OA$(n, m, 2)$, the OofA-OA$(24, 5, 3)$ in Table 8 is unique up to isomorphism. Not surprisingly, it has the form in (4), that is, it corresponds to a foldover design. Fourth, Schoen and Mee (2023) recommended 12 Pareto-optimal OofA-OA$(24, 7, 2)$'s. My proposal in Table 8 is different from theirs. Fifth, by Theorem 3, ranking results according to the centralized generalized wordlength patterns are consistent with those according to the generalized wordlength patterns. In other words, all optimal order-of-addition orthogonal arrays in Table 8 have minimum G_2-aberration. Therefore, when these order-of-addition orthogonal arrays are used to design order-of-addition experiments, the main effects can be estimated with optimal efficiency in the first-stage analysis. Based on the theoretical results developed by Cheng, Deng and Tang (2002), all main effects and some two-factor interaction effects can also be estimated efficiently in the second-stage analysis.

Table 8: Optimal order-of-addition orthogonal arrays.

m	n	t	$C_1(\mathcal{V})$	$C_2(\mathcal{V})$	$C_3(\mathcal{V})$	$C_4(\mathcal{V})$	$C_5(\mathcal{V})$	$C_6(\mathcal{V})$	ID	Source
4	12	2	0.000	0.000	1.333	0.000	1.333	0.000	1	Voelkel (2019)
4	24	6	0.000	0.000	0.000	0.000	0.000	0.000	10	Schoen and Mee (2023)
5	12	2	0.000	0.000	11.111	11.911	20.889	18.844	1	Zhao, Lin and Liu (2022)
5	24	3	0.000	0.000	0.000	11.911	0.000	18.844	8640	Schoen and Mee (2023)
6	24	2	0.000	0.000	11.556	44.578	124.889	191.067	14503	Schoen and Mee (2023)
7	24	2	0.000	0.000	47.444	190.133	881.889	2121.257	218	Schoen and Mee (2023)

4 Concluding Remarks

Some existing theoretical results developed for two-level orthogonal arrays may not hold for order-of-addition orthogonal arrays due to the fact that some J-characteristics of $Z_{\mathcal{U},\mathcal{Q}}$ are not equal to zero. Because the full design contains the most comprehensive information regarding the treatment-response relationship, $Z_{\mathcal{U},\mathcal{Q}}$ can be used as a common reference when evaluating a fractional design or comparing two fractional designs. A series of numerical indices called centralized generalized wordlength pattern is proposed in this paper to implement this simple idea. Specifically, it is designed to quantify the similarity between $Z_{\mathcal{V},\mathcal{Q}}$ and $Z_{\mathcal{U},\mathcal{Q}}$ when projecting onto various numbers of pairwise order factors. Based on the centralized generalized wordlength pattern, some new results are further developed to characterize and compare order-of-addition orthogonal arrays. The functional relationship between the centralized and non-centralized generalized wordlength patterns is further simplified to reach the conclusion that they yield consistent ranking results.

The centralized generalized wordlength pattern takes into account several combinatorial and statistical properties that may help experimental data analysis. In the first-stage analysis, suppose that the following main effects model of the pairwise order factors is used to fit the observed data:

$$y_n = \gamma_0 1_n + Z_{\mathcal{V},\mathcal{Q}}\gamma_1 + \epsilon_n,$$

where y_n denotes the $n \times 1$ response vector, γ_0 represents the overall mean, γ_1 denotes the $q \times 1$ vector of all main effects of the pairwise order factors, and ϵ_n represents the $n \times 1$ vector of error terms. All error terms in ϵ_n are assumed to be uncorrelated random variables with zero mean and constant variance. Let $\hat{\gamma}_0$ and $\hat{\gamma}_1$ denote the least squares estimators of γ_0 and γ_1. The centralized generalized wordlength pattern summarizes the following properties.

(A) Balanced property: if $C_1(\mathcal{V}) = 0$, then $\hat{\gamma}_0$ and $\hat{\gamma}_1$ are uncorrelated and they can also be inferred independently under the assumption of normality.

(B) Optimality property: if $C_1(\mathcal{V}) = C_2(\mathcal{V}) = 0$, then $\hat{\gamma}_0$ and $\hat{\gamma}_1$ achieve optimal estimation efficiency over all pairwise order matrices of the same order.

(C) Robustness property: if $C_1(\mathcal{V}) = C_2(\mathcal{V}) = C_3(\mathcal{V}) = 0$, then $\hat{\gamma}_1$ is still unbiased even when some two-factor interaction effects are not negligible.

Actually, the three properties have also been verified by Voelkel (2019), Peng, Mukerjee and Lin (2019) and Mee (2020), respectively. These properties help researchers to get more reliable results of experimental data analysis. In particular, as shown in Example 8, the condition $C_2(\mathcal{V}) = 0$ is not really necessary for the robustness property in (C). It is deliberately added to legitimatize the sequential minimization procedure for the centralized generalized wordlength pattern. Based on Theorem 3, the theoretical results developed by Cheng, Deng and Tang (2002) can also be used to support the centralized generalized wordlength pattern. Specifically, when comparing order-of-addition orthogonal arrays, it tends to yield highly efficient designs for estimating all main effects and some two-factor interaction effects in the second-stage analysis.

Although the centralized and non-centralized generalized wordlength patterns appear similar, there are still some differences when comparing pairwise order matrices. Suppose that an order-of-addition orthogonal array of strength two $Z_{\mathcal{V},\mathcal{Q}}$ is used to design an order-of-addition experiment. Let $E_{\mathcal{V},\mathcal{S}_a}$ denote the $n \times s_a$ submatrix of $E_{\mathcal{V},\mathcal{W}}$ consisting of all column vectors indexed by $\mathcal{S}_a = \{\mathcal{W}_d : |\mathcal{W}_d| = a\}$, where $s_a = |\mathcal{S}_a| = q!/[a!(q-a)!]$. Assume that the expectation of y_n has the form

$$\mathbb{E}(y_n) = E_{\mathcal{V},\mathcal{S}_0}\gamma_0 + E_{\mathcal{V},\mathcal{S}_1}\gamma_1 + E_{\mathcal{V},\mathcal{S}_2}\gamma_2 + \cdots + E_{\mathcal{V},\mathcal{S}_q}\gamma_q,$$

where γ_a denotes the $s_a \times 1$ vector of a-way interaction effects. Note that $E_{\mathcal{V},\mathcal{S}_0} = 1_n$ and $E_{\mathcal{V},\mathcal{S}_1} = Z_{\mathcal{V},\mathcal{Q}}$. The expectation of the least squares estimator of γ_1 has the form

$$\mathbb{E}(\hat{\gamma}_1) = \gamma_1 + K_2\gamma_2 + \cdots + K_q\gamma_q,$$

where $K_a = (Z_{\mathcal{V},\mathcal{Q}}^\top Z_{\mathcal{V},\mathcal{Q}})^{-1} Z_{\mathcal{V},\mathcal{Q}}^\top E_{\mathcal{V},\mathcal{S}_a}$ for $a = 2, 3, \ldots, q$. Tang and Deng (1999) showed that sequentially minimizing $A_3(\mathcal{V}), A_4(\mathcal{V}), \ldots, A_q(\mathcal{V})$ is equivalent to sequentially minimizing $\|K_2\|^2, \|K_3\|^2, \ldots, \|K_{q-1}\|^2$ when evaluating two-level orthogonal arrays of strength two. Note that $\|\cdot\|^2$ denotes the squared L_2-norm.

This important result provides a statistical justification for the minimum G_2-aberration criterion. That is, it tends to sequentially minimize the contaminations of non-negligible interaction effects on the estimation of main effects in the first-stage analysis. However, this conclusion does not hold for order-of-addition orthogonal arrays of strength two because they are not column-orthogonal.

The centralized generalized wordlength pattern is proposed in order to describe the pairwise order matrix of an order-of-addition design more comprehensively. An immediate application is to further discriminate between two candidate designs that perform equally well under a conventional criterion. In addition to characterizing and comparing existing designs, some results of this paper can also be used to develop construction methods for generating new designs. There are at least two promising directions to pursue. Firstly, Xu (2002) developed an algorithm by using the J-characteristics to generate efficient factorial designs. Based on Corollary 1, it seems possible to modify his algorithm to generate efficient order-of-addition designs. Secondly, based on Corollary 4 and Proposition 3, an order-of-addition orthogonal array of strength two can be obtained by searching for an index set $\mathcal{V}$ from $\mathcal{U}$ such that $A_1(\mathcal{V}) = 0$ and $A_2(\mathcal{V}) = m(m-1)(m-2)/18$. On the other hand, the centralized and non-centralized generalized wordlength patterns are legitimate numerical indices only for the main effects model of the pairwise order factors. It is currently not clear whether or not the obtained designs in Table 8 are still good designs under other statistical models or optimality criteria. Developing a model-free criterion can be practical to generate such robust order-of-addition designs. Recently, Huang and Yang (2025) proposed a distance-based criterion to generate maximin distance order-of-addition designs. Interestingly, as shown in Section 3.3, the centralized and non-centralized generalized wordlength patterns can also be obtained using the distance distributions of $Z_{\mathcal{V},\mathcal{Q}}$ and $Z_{\mathcal{U},\mathcal{Q}}$. Based on Proposition 1, it seems possible to develop a distance-based criterion to compare $Z_{\mathcal{V},\mathcal{Q}}$ and $Z_{\mathcal{U},\mathcal{Q}}$ such that more model-free order-of-addition designs can be generated for future work. These interesting topics may be worth pursuing in future research.

Supplementary Materials

Supplementary materials of this paper include the following sections.

(S1) Some values of $A_a(\mathcal{U})$

(S2) Design matrix of an OofA-OA$(48, 9, 2)$

(S3) Code

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Appendix: Proofs of Theorems

A.1 Proof of Proposition 1

Proof. Let $D_k(g,\mathcal{U})$ denote the number of pairwise order vectors that have k entries different from $z_{g,\mathcal{Q}}$ given by

$$D_k(g,\mathcal{U}) = |\{z_{h,\mathcal{Q}} : d_H(z_{g,\mathcal{Q}}, z_{h,\mathcal{Q}}) = k \text{ and } h \in \mathcal{U}\}|.$$

Because $d_H(z_{1,\mathcal{Q}}, z_{h,\mathcal{Q}}) = d_H(1_q, z_{h,\mathcal{Q}}) = inv(t_h)$, one has

$$\begin{aligned} D_k(1,\mathcal{U}) &= |\{z_{h,\mathcal{Q}} : d_H(z_{1,\mathcal{Q}}, z_{h,\mathcal{Q}}) = k \text{ and } h \in \mathcal{U}\}| \\ &= |\{z_{h,\mathcal{Q}} : d_H(1_q, z_{h,\mathcal{Q}}) = k \text{ and } h \in \mathcal{U}\}| \\ &= |\{t_h : inv(t_h) = k \text{ and } h \in \mathcal{U}\}| \\ &= b(m,k) \end{aligned}$$

for $k = 0, 1, \ldots, q$. Based on Lemma A1 of Peng, Mukerjee and Lin (2019), for every $g \in \mathcal{U}$, there exists a signed permutation matrix P such that

$$\begin{aligned} P^\top z_{g,\mathcal{Q}} &= z_{1,\mathcal{Q}} \\ &= 1_q. \end{aligned}$$

Because $Z_{\mathcal{U},\mathcal{Q}}$ is unique up to isomorphism, one has

$$\begin{aligned} D_k(g,\mathcal{U}) &= |\{z_{h,\mathcal{Q}} : d_H(z_{g,\mathcal{Q}}, z_{h,\mathcal{Q}}) = k \text{ and } h \in \mathcal{U}\}| \\ &= |\{z_{h,\mathcal{Q}} : d_H\left(P^\top z_{g,\mathcal{Q}}, P^\top z_{h,\mathcal{Q}}\right) = k \text{ and } h \in \mathcal{U}\}| \\ &= |\{z_{h,\mathcal{Q}} : d_H(1_q, z_{h,\mathcal{Q}}) = k \text{ and } h \in \mathcal{U}\}| \\ &= D_k(1,\mathcal{U}) \end{aligned}$$

for every $g \in \mathcal{U}$. Therefore, one has

$$\begin{aligned} B_k(\mathcal{U}) &= \frac{1}{N}|\{(z_{g,\mathcal{Q}}, z_{h,\mathcal{Q}}) : d_H(z_{g,\mathcal{Q}}, z_{h,\mathcal{Q}}) = k \text{ and } g, h \in \mathcal{U}\}| \\ &= \frac{1}{N}\sum_{g=1}^{N} D_k(g,\mathcal{U}) \\ &= \frac{N}{N} D_k(1,\mathcal{U}) \\ &= b(m,k) \end{aligned}$$

for $k = 0, 1, \ldots, q$. This completes the proof. □

A.2 Proof of Corollary 1

Proof. Given the pairwise order matrix $Z_{\mathcal{U},\mathcal{Q}}$, let $Z_{\mathcal{I},\mathcal{Q}}$ denote the $(2^q - N) \times q$ matrix consisting of all invalid pairwise order vectors as row vectors, where $\mathcal{I} = \{N+1, N+2, \ldots, 2^q\}$ is the index set of all invalid pairwise order vectors. The juxtaposition of $Z_{\mathcal{U},\mathcal{Q}}$ and $Z_{\mathcal{I},\mathcal{Q}}$ given by

$$\begin{bmatrix} Z_{\mathcal{U},\mathcal{Q}} \\ Z_{\mathcal{I},\mathcal{Q}} \end{bmatrix}$$

consists of 2^q $(+1,-1)$-vectors of length q as row vectors. Let $E_{\mathcal{I},\mathcal{W}}$ represent the $(2^q - N) \times 2^q$ matrix given by

$$E_{\mathcal{I},\mathcal{W}} = \left[\begin{array}{cccc} e_{\mathcal{I},1} & e_{\mathcal{I},2} & \cdots & e_{\mathcal{I},2^q} \end{array} \right].$$

The dth column vector of $E_{\mathcal{I},\mathcal{W}}$ has the form $e_{\mathcal{I},d} = \odot_{ij \in \mathcal{W}_d} z_{\mathcal{I},ij}$, where $z_{\mathcal{I},ij}$ denotes the $(2^q - N) \times 1$ vector consisting all pairwise order factors of components i and j indexed by $\mathcal{I}$. The juxtaposition of $E_{\mathcal{U},\mathcal{W}}$ and $E_{\mathcal{I},\mathcal{W}}$ given by

$$H = \left[\begin{array}{c} E_{\mathcal{U},\mathcal{W}} \\ E_{\mathcal{I},\mathcal{W}} \end{array} \right]$$

is a Hadamard matrix of order 2^q and it is isomorphic to that in (5) of Tang (2001). Note that two Hadamard matrices are said to be isomorphic if one can be obtained from the other by interchanging row vectors, interchanging column vectors, sign-switching a row vector or a column vector, or a combination of these operations. Based on Theorem 1 of Tang (2001), one has

$$\left[\begin{array}{c} n_{\mathcal{V}} \\ 0_{2^q - N} \end{array} \right] = \frac{1}{2^q} H J_{\mathcal{V}},$$

where $n_{\mathcal{V}}$ represents the $N \times 1$ vector consisting of $n_1, n_2, \ldots, n_N$, and $0_{2^q - N}$ denotes the $(2^q - N) \times 1$ zero vector. Note that n_h denotes the number of observations of t_h. Because H is invertible, $n_{\mathcal{V}}$ is uniquely determined by $J_{\mathcal{V}}$. This completes the proof. □

A.3 Proof of Proposition 2

Basically, the proof of Proposition 2 is established by similar arguments to those of Proposition 3 of Deng and Tang (1999) and Proposition 1 of Deng and Tang (2002). Some minor changes are made to take the combinatorial properties of order-of-addition orthogonal arrays into account.

Proof of conclusion (a). Let $Z_{\mathcal{V},\mathcal{Q}}$ denote an OofA-OA$(n, m, 2)$ for $m \geq 4$. Voelkel (2019) noted that n must be a multiple of 12, denoted by $n = 12u$, where u is a positive integer. Based on Theorem 2 of Peng, Mukerjee and Lin (2019), one has $J_{\mathcal{W}_d}(\mathcal{V}) = 0$ for every $\mathcal{W}_d$ with $|\mathcal{W}_d| = 1$ and $J_{\mathcal{W}_d}(\mathcal{V})$ is equal to zero or $\pm n/3 = \pm 4u$ for every $\mathcal{W}_d$ with $|\mathcal{W}_d| = 2$. Therefore, the value of $J_{\mathcal{W}_d}(\mathcal{V})$ is a multiple of four for every $\mathcal{W}_d$ with $|\mathcal{W}_d| \leq 2$. Suppose that $J_{\mathcal{W}_d}(\mathcal{V})$ is a multiple of four for an arbitrary $\mathcal{W}_d$ with $|\mathcal{W}_d| \leq k$, that is, $J_{\mathcal{W}_d}(\mathcal{V}) = 4v$, where v is an integer. Because $n = 12u$ and $J_{\mathcal{W}_d}(\mathcal{V}) = 4v$, the two numbers $+1$ and -1 appear $6u + 2v$ times and $6u - 2v$ times in $e_{\mathcal{V},d}$, respectively, where $e_{\mathcal{V},d} = \odot_{ij \in \mathcal{W}_d} z_{\mathcal{V},ij}$. Let M represent the $n \times 2$ matrix consisting of $e_{\mathcal{V},d}$ and $z_{\mathcal{V},ij}$ as column vectors, where $ij \in \mathcal{Q} \setminus \mathcal{W}_d$. Because $Z_{\mathcal{V},\mathcal{Q}}$ is an OofA-OA$(n, m, 2)$, the two numbers $+1$ and -1 also occur equally often in $z_{\mathcal{V},ij}$. Let f denote the number of times that the ordered pair $(-1,-1)$ occurs in the row vectors of M. It is not difficult to see that the numbers of times that the ordered pairs $(-1,+1)$, $(+1,-1)$ and $(+1,+1)$ occur in the row vectors of M are equal to $6u - 2v - f$, $6u - f$ and $2v + f$. The frequency distribution of $(+1,-1)$-vectors of length two in M is summarized in Table A1, where $e_{h,d}$ and $z_{h,ij}$ are entries of $e_{\mathcal{V},d}$ and $z_{\mathcal{V},ij}$, respectively.

Table A1: Frequency distribution of $(+1, -1)$-vectors of length two in M.

$e_{h,d}$	$z_{h,ij}$	Frequency
-1	-1	f
-1	$+1$	$6u - 2v - f$
$+1$	-1	$6u - f$
$+1$	$+1$	$2v + f$
Total		$12u$

Based on Table A1, the J-characteristic of $Z_{\mathcal{V},\mathcal{Q}}$ corresponding to $\mathcal{W}_c$, where $\mathcal{W}_c = \mathcal{W}_d \cup \{ij\}$ and $|\mathcal{W}_c| = k+1$, is given by

$$\begin{aligned} J_{\mathcal{W}_c}(\mathcal{V}) &= e_{\mathcal{V},d}^{\top} z_{\mathcal{V},ij} \\ &= f - (6u - 2v - f) - (6u - f) + (2v + f) \\ &= 4(f - 3u + v). \end{aligned}$$

Obviously, $J_{\mathcal{W}_c}(\mathcal{V})$ is a multiple of four for every $\mathcal{W}_c$ with $|\mathcal{W}_c| = k+1$. The statement is proven by induction. □

Proof of conclusion (b). Let $Z_{\mathcal{V},\mathcal{Q}}$ denote an OofA-OA$(n, m, 2)$, where $n = 24u$ and u is a positive integer. Based on Theorem 2 of Peng, Mukerjee and Lin (2019), one has $J_{\mathcal{W}_d}(\mathcal{V}) = 0$ for every $\mathcal{W}_d$ with $|\mathcal{W}_d| = 1$ and $J_{\mathcal{W}_d}(\mathcal{V})$ is either equal to zero or $\pm n/3 = \pm 8u$ for every $\mathcal{W}_d$ with $|\mathcal{W}_d| = 2$. Therefore, the value of $J_{\mathcal{W}_d}(\mathcal{V})$ is a multiple of eight for every $\mathcal{W}_d$ with $|\mathcal{W}_d| \leq 2$. Suppose that $J_{\mathcal{W}_d}(\mathcal{V})$ is a multiple of eight for an arbitrary $\mathcal{W}_d$ with $|\mathcal{W}_d| \leq k$, that is, $J_{\mathcal{W}_d}(\mathcal{V}) = 8v$, where v is an integer. Let $\mathcal{W}_c$ denote an arbitrary subset of $\mathcal{Q}$ with $|\mathcal{W}_c| = k+1$. In addition, let $\mathcal{W}_a$ and $\mathcal{W}_b$ represent two subsets of $\mathcal{W}_c$ with $|\mathcal{W}_a| = |\mathcal{W}_b| = 1$. Define M as the $n \times 3$ matrix consisting of $e_{\mathcal{V},a} = \odot_{ij \in \mathcal{W}_a} z_{\mathcal{V},ij}$, $e_{\mathcal{V},b} = \odot_{ij \in \mathcal{W}_b} z_{\mathcal{V},ij}$ and $e_{\mathcal{V},c} = \odot_{ij \in \mathcal{W}_c} z_{\mathcal{V},ij}$ as column vectors. The frequency distribution of $(+1, -1)$-vectors of length three in M is summarized in Table A2, where f_i and $u_j - f_i$ are non-negative integers. Note also that $u_1 + u_2 = n/2$.

Table A2: Frequency distribution of $(+1, -1)$-vectors of length three in M.

$e_{h,a}$	$e_{h,b}$	$e_{h,c}$	Frequency
-1	-1	-1	f_1
-1	-1	$+1$	$u_1 - f_1$
-1	$+1$	-1	f_2
-1	$+1$	$+1$	$u_2 - f_2$
$+1$	-1	-1	f_3
$+1$	-1	$+1$	$u_2 - f_3$
$+1$	$+1$	-1	f_4
$+1$	$+1$	$+1$	$u_1 - f_4$
Total			$2(u_1 + u_2)$

Based on the frequency distribution in Table A2, the J-characteristics of $Z_{\mathcal{V},\mathcal{Q}}$ corresponding to $\mathcal{W}_c$, $\mathcal{W}_c \setminus \mathcal{W}_a$, $\mathcal{W}_c \setminus \mathcal{W}_b$ and $\mathcal{W}_c \setminus (\mathcal{W}_a \cup \mathcal{W}_b)$ are given by

$$J_{\mathcal{W}_c}(\mathcal{V}) = -2f_1 - 2f_2 - 2f_3 - 2f_4 + 2u_1 + 2u_2,$$

$$\begin{aligned} J_{\mathcal{W}_c\setminus\mathcal{W}_a}(\mathcal{V}) &= 2f_1+2f_2-2f_3-2f_4, \\ J_{\mathcal{W}_c\setminus\mathcal{W}_b}(\mathcal{V}) &= 2f_1-2f_2+2f_3-2f_4, \\ J_{\mathcal{W}_c\setminus(\mathcal{W}_a\cup\mathcal{W}_b)}(\mathcal{V}) &= -2f_1+2f_2+2f_3-2f_4+2u_1-2u_2, \end{aligned}$$

respectively. Because

$$J_{\mathcal{W}_c}(\mathcal{V})+J_{\mathcal{W}_c\setminus\mathcal{W}_a}(\mathcal{V})+J_{\mathcal{W}_c\setminus\mathcal{W}_b}(\mathcal{V})+J_{\mathcal{W}_c\setminus(\mathcal{W}_a\cup\mathcal{W}_b)}(\mathcal{V})=4u_1-8f_4,$$

one has

$$J_{\mathcal{W}_c}(\mathcal{V})=4u_1-8f_4-J_{\mathcal{W}_c\setminus\mathcal{W}_a}(\mathcal{V})-J_{\mathcal{W}_c\setminus\mathcal{W}_b}(\mathcal{V})-J_{\mathcal{W}_c\setminus(\mathcal{W}_a\cup\mathcal{W}_b)}(\mathcal{V}).$$

Because $Z_{\mathcal{V},\mathcal{Q}}$ is an OofA-OA$(n,m,2)$, Voelkel (2019) noted that the ordered pair (u_1,u_2) must have the following values:

$$(u_1,u_2)=\begin{cases} (n/3,n/6) & \text{if } i=k, j\neq l \text{ or } i\neq k,\ j=l; \\ (n/6,n/3) & \text{if } i=l \text{ or } j=k; \\ (n/4,n/4) & \text{otherwise.} \end{cases}$$

Therefore, if $n=24u$, then

$$J_{\mathcal{W}_c}(\mathcal{V})=\begin{cases} 32u-8f_4-J_{\mathcal{W}_c\setminus\mathcal{W}_a}(\mathcal{V})-J_{\mathcal{W}_c\setminus\mathcal{W}_b}(\mathcal{V})-J_{\mathcal{W}_c\setminus(\mathcal{W}_a\cup\mathcal{W}_b)}(\mathcal{V}) & \text{if } u_1=n/3; \\ 16u-8f_4-J_{\mathcal{W}_c\setminus\mathcal{W}_a}(\mathcal{V})-J_{\mathcal{W}_c\setminus\mathcal{W}_b}(\mathcal{V})-J_{\mathcal{W}_c\setminus(\mathcal{W}_a\cup\mathcal{W}_b)}(\mathcal{V}) & \text{if } u_1=n/6; \\ 24u-8f_4-J_{\mathcal{W}_c\setminus\mathcal{W}_a}(\mathcal{V})-J_{\mathcal{W}_c\setminus\mathcal{W}_b}(\mathcal{V})-J_{\mathcal{W}_c\setminus(\mathcal{W}_a\cup\mathcal{W}_b)}(\mathcal{V}) & \text{if } u_1=n/4. \end{cases}$$

Because $|\mathcal{W}_c\setminus\mathcal{W}_a|=|\mathcal{W}_c\setminus\mathcal{W}_b|=k$ and $|\mathcal{W}_c\setminus(\mathcal{W}_a\cup\mathcal{W}_b)|=k-1$, one has $J_{\mathcal{W}_c\setminus\mathcal{W}_a}(\mathcal{V})$, $J_{\mathcal{W}_c\setminus\mathcal{W}_b}(\mathcal{V})$ and $J_{\mathcal{W}_c\setminus(\mathcal{W}_a\cup\mathcal{W}_b)}(\mathcal{V})$ are all multiples of eight, with the result that $J_{\mathcal{W}_c}(\mathcal{V})$ is also a multiple of eight for every $\mathcal{W}_c$ with $|\mathcal{W}_c|=k+1$. The statement is proven by induction. □

A.4 Proof of Theorem 1

Proof. Suppose that $Z_{\mathcal{V},\mathcal{Q}}$ is an OofA-OA(n,m,t). It is straightforward to see that $J_{\mathcal{W}_d}(\mathcal{V})/n=J_{\mathcal{W}_d}(\mathcal{U})/N$ for every $\mathcal{W}_d$ with $|\mathcal{W}_d|\leq t$. Conversely, suppose that $J_{\mathcal{W}_d}(\mathcal{V})/n=J_{\mathcal{W}_d}(\mathcal{U})/N$ for every $\mathcal{W}_d$ with $|\mathcal{W}_d|=a\leq t$. Given an arbitrary $\mathcal{W}_d$ with $|\mathcal{W}_d|=a\leq t$, the $n\times a$ submatrix of $Z_{\mathcal{V},\mathcal{Q}}$, denoted by $Z_{\mathcal{V},\mathcal{W}_d}$, can be obtained by deleting the pairwise order factors indexed by $\mathcal{Q}\setminus\mathcal{W}_d$ from $Z_{\mathcal{V},\mathcal{Q}}$. Similarly, the $N\times a$ submatrix of $Z_{\mathcal{U},\mathcal{Q}}$, denoted by $Z_{\mathcal{U},\mathcal{W}_d}$, can be obtained by deleting the pairwise order factors indexed by $\mathcal{Q}\setminus\mathcal{W}_d$ from $Z_{\mathcal{U},\mathcal{Q}}$. Let $J^*_{\mathcal{V}}$ and $J^*_{\mathcal{U}}$ denote the $2^a\times 1$ vectors consisting of all J-characteristics of $Z_{\mathcal{V},\mathcal{W}_d}$ and $Z_{\mathcal{U},\mathcal{W}_d}$, respectively. In addition, let $n^*_{\mathcal{V}}$ and $n^*_{\mathcal{U}}$ represent $R\times 1$ vectors consisting of the numbers of times that the R valid pairwise order vectors of length a occur in $Z_{\mathcal{V},\mathcal{W}_d}$ and $Z_{\mathcal{U},\mathcal{W}_d}$, respectively. Note that the number of valid pairwise order vectors R is determined by $\mathcal{W}_d$. By similar arguments of the proof of Corollary 1, one has

$$\begin{bmatrix} n^*_{\mathcal{V}} \\ 0_{2^a-R} \end{bmatrix}=\frac{1}{2^a}H^*J^*_{\mathcal{V}},$$

and

$$\begin{bmatrix} n^*_{\mathcal{U}} \\ 0_{2^a-R} \end{bmatrix}=\frac{1}{2^a}H^*J^*_{\mathcal{U}},$$

where H^* is a Hadamard matrix of order 2^a. Based on these facts, one has

$$\begin{aligned} \begin{bmatrix} n^*_{\mathcal{V}} \\ 0_{2^a-R} \end{bmatrix} &= \frac{1}{2^a} H^* J^*_{\mathcal{V}} \\ &= \frac{1}{2^a} H^* \left(\frac{n}{N} J^*_{\mathcal{U}}\right) \\ &= \frac{n}{N} \left(\frac{1}{2^a} H^* J^*_{\mathcal{U}}\right) \\ &= \frac{n}{N} \begin{bmatrix} n^*_{\mathcal{U}} \\ 0_{2^a-R} \end{bmatrix}. \end{aligned}$$

By definition, $Z_{\mathcal{V},\mathcal{Q}}$ is an OofA-OA(n, m, t). This completes the proof. □

A.5 Proof of Theorem 2

Proof. Given a foldover design, it is straightforward to see that $e_{\mathcal{G},d} = -e_{\mathcal{H},d}$ for every $\mathcal{W}_d$ with odd $|\mathcal{W}_d|$. The J-characteristic of $Z_{\mathcal{V},\mathcal{Q}}$ corresponding to $\mathcal{W}_d$ is given by

$$\begin{aligned} J_{\mathcal{W}_d}(\mathcal{V}) &= e^{\top}_{\mathcal{V},d} 1_n \\ &= e^{\top}_{\mathcal{H},d} 1_{n/2} + e^{\top}_{\mathcal{G},d} 1_{n/2} \\ &= e^{\top}_{\mathcal{H},d} 1_{n/2} - e^{\top}_{\mathcal{H},d} 1_{n/2} \\ &= 0. \end{aligned}$$

Based on Lemma A1 of Cheng, Mee and Yee (2008), the converse statement is also true. □

A.6 Proof of Corollary 3

Proof. Based on Theorem 2, if the submatrix $Z_{\mathcal{H},\mathcal{Q}}$ in (4) is an OofA-OA(n, m, t) and t is even, then $J_{\mathcal{W}_d}(\mathcal{V}) = J_{\mathcal{W}_d}(\mathcal{U}) = 0$ for every $\mathcal{W}_d$ with $|\mathcal{W}_d| = t + 1$ and $t + 1$ is odd such that $C_{t+1}(\mathcal{V}) = 0$. By Corollary 2, the corresponding pairwise order matrix $Z_{\mathcal{V},\mathcal{Q}}$ in (4) is an OofA-OA$(2n, m, t + 1)$. □

A.7 Proof of Theorem 3

Proof of part (a). Based on Theorem 2, because $\mathcal{T}$ is a foldover design, one has $J_{\mathcal{W}_d}(\mathcal{U}) = 0$ for every $\mathcal{W}_d$ with odd $|\mathcal{W}_d|$ such that

$$C_a(\mathcal{V}) = A_a(\mathcal{V})$$

for every odd a. Let $E_{\mathcal{U},\mathcal{S}_a}$ denote the $N \times s_a$ submatrix of $E_{\mathcal{U},\mathcal{W}}$ consisting of all column vectors indexed by $\mathcal{S}_a = \{\mathcal{W}_d : |\mathcal{W}_d| = a\}$, where $s_a = |\mathcal{S}_a| = q!/[a!(q - a)!]$. By Corollary 1, because

$$\begin{aligned} J_{\mathcal{V}} &= H^{\top} \begin{bmatrix} n_{\mathcal{V}} \\ 0_{2^q-N} \end{bmatrix} \\ &= E^{\top}_{\mathcal{U},\mathcal{W}} n_{\mathcal{V}}, \end{aligned}$$

one has

$$\frac{1}{n}\sum_{|\mathcal{W}_d|=a} J_{\mathcal{W}_d}(\mathcal{V})J_{\mathcal{W}_d}(\mathcal{U}) - \frac{1}{N}\sum_{|\mathcal{W}_d|=a}[J_{\mathcal{W}_d}(\mathcal{U})]^2 = \frac{1}{n}n_{\mathcal{V}}^\top E_{\mathcal{U},\mathcal{S}_a}E_{\mathcal{U},\mathcal{S}_a}^\top 1_N - \frac{1}{N}1_N^\top E_{\mathcal{U},\mathcal{S}_a}E_{\mathcal{U},\mathcal{S}_a}^\top 1_N$$
$$= \left(\frac{1}{n}n_{\mathcal{V}}^\top - \frac{1}{N}1_N^\top\right)E_{\mathcal{U},\mathcal{S}_a}E_{\mathcal{U},\mathcal{S}_a}^\top 1_N. \quad \text{(A1)}$$

Let $e_{1,\mathcal{S}_a}^\top$ denote the first row vector of $E_{\mathcal{U},\mathcal{S}_a}$. Because $e_{1,\mathcal{S}_a}$ is determined by t_1, one has $e_{1,\mathcal{S}_a}^\top = 1_{s_a}^\top$. The row sum of the first row vector of $E_{\mathcal{U},\mathcal{S}_a}E_{\mathcal{U},\mathcal{S}_a}^\top$ is equal to

$$\begin{aligned} e_{1,\mathcal{S}_a}^\top E_{\mathcal{U},\mathcal{S}_a}^\top 1_N &= 1_{s_a}^\top E_{\mathcal{U},\mathcal{S}_a}^\top 1_N \\ &= \sum_{|\mathcal{W}_d|=a} J_{\mathcal{W}_d}(\mathcal{U}). \end{aligned}$$

Actually, every row vector of $E_{\mathcal{U},\mathcal{S}_a}E_{\mathcal{U},\mathcal{S}_a}^\top$ has row sum $\sum_{|\mathcal{W}_d|=a} J_{\mathcal{W}_d}(\mathcal{U})$ due to the fact that every row vector of $E_{\mathcal{U},\mathcal{S}_a}E_{\mathcal{U},\mathcal{S}_a}^\top$ consists of the same set of entries as its first row vector. The right-hand-side term of (A1) can then be expressed as

$$\begin{aligned} \sum_{|\mathcal{W}_d|=a} J_{\mathcal{W}_d}(\mathcal{U})\left(\frac{1}{n}n_{\mathcal{V}}^\top - \frac{1}{N}1_N^\top\right)1_N &= \sum_{|\mathcal{W}_d|=a} J_{\mathcal{W}_d}(\mathcal{U})\left(\frac{n}{n} - \frac{N}{N}\right) \\ &= 0, \end{aligned}$$

with the result that

$$\frac{1}{n}\sum_{|\mathcal{W}_d|=a} J_{\mathcal{W}_d}(\mathcal{V})J_{\mathcal{W}_d}(\mathcal{U}) = \frac{1}{N}\sum_{|\mathcal{W}_d|=a}[J_{\mathcal{W}_d}(\mathcal{U})]^2.$$

Therefore, for every even a, $C_a(\mathcal{V})$ can be expressed as

$$\begin{aligned} C_a(\mathcal{V}) &= \sum_{|\mathcal{W}_d|=a}\left[\frac{1}{n}J_{\mathcal{W}_d}(\mathcal{V}) - \frac{1}{N}J_{\mathcal{W}_d}(\mathcal{U})\right]^2 \\ &= \sum_{|\mathcal{W}_d|=a}\left[\frac{1}{n}J_{\mathcal{W}_d}(\mathcal{V})\right]^2 - \frac{2}{nN}\sum_{|\mathcal{W}_d|=a}J_{\mathcal{W}_d}(\mathcal{V})J_{\mathcal{W}_d}(\mathcal{U}) + \sum_{|\mathcal{W}_d|=a}\left[\frac{1}{N}J_{\mathcal{W}_d}(\mathcal{U})\right]^2 \\ &= \sum_{|\mathcal{W}_d|=a}\left[\frac{1}{n}J_{\mathcal{W}_d}(\mathcal{V})\right]^2 - \sum_{|\mathcal{W}_d|=a}\left[\frac{1}{N}J_{\mathcal{W}_d}(\mathcal{U})\right]^2 \\ &= A_a(\mathcal{V}) - A_a(\mathcal{U}). \end{aligned}$$

This completes the proof. □

Proof of part (b). By Corollary 1, because

$$J_{\mathcal{V}} = H^\top \begin{bmatrix} n_{\mathcal{V}} \\ 0_{2^q-N} \end{bmatrix},$$

where $H^\top H = HH^\top = 2^q I_{2^q}$, one has

$$\begin{aligned} \sum_{a=1}^{q} A_a(\mathcal{V}) &= \frac{1}{n^2}J_{\mathcal{V}}^\top J_{\mathcal{V}} - 1 \\ &= \frac{2^q}{n^2}\sum_{h=1}^{N} n_h^2 - 1. \end{aligned}$$

Similarly, one has $\sum_{a=1}^{q} A_a(\mathcal{U}) = 2^q/N - 1$, where $A_a(\mathcal{U}) = 0$ for odd a. Because $C_a(\mathcal{V}) = A_a(\mathcal{V}) - A_a(\mathcal{U})$, one has

$$\begin{aligned}\sum_{a=1}^{q} C_a(\mathcal{V}) &= \sum_{a=1}^{q} A_a(\mathcal{V}) - \sum_{a=1}^{q} A_a(\mathcal{U}) \\ &= 2^q \left(\frac{1}{n^2} \sum_{h=1}^{N} n_h^2 - \frac{1}{N} \right).\end{aligned}$$

This completes the proof. □

A.8 Proof of Proposition 3

Proof of part (a). Based on Theorem 2 of Peng, Mukerjee and Lin (2019), one has $J_{\mathcal{W}_d}(\mathcal{U})/N = 0$ or $\pm 1/3$ for every $\mathcal{W}_d$ with $|\mathcal{W}_d| = 2$. Because there are $m(m-1)(m-2)/2$ non-zero normalized J-characteristics, one has $A_2(\mathcal{U}) = m(m-1)(m-2)/18$. This completes the proof. □

Proof of part (b). By Theorem 2, when q is odd, $A_q(\mathcal{U}) = 0$. Because $k!/[j!(k-j)!] = 0$ for every $k < j$ and $(q-k)!/[(q-j)!(j-k)!] = 0$ for every $k > j$, one has

$$\binom{k}{j}\binom{q-k}{q-j} = \begin{cases} 1 & \text{if } j = k; \\ 0 & \text{otherwise.} \end{cases}$$

The qth Krawtchouk polynomial has the following two values:

$$\begin{aligned}P_q(k, q, 2) &= \sum_{j=0}^{q} (-1)^j \binom{k}{j}\binom{q-k}{q-j} \\ &= \begin{cases} +1 & \text{if } j = k \text{ is even;} \\ -1 & \text{if } j = k \text{ is odd.} \end{cases}\end{aligned}$$

Because $F_m(-1) = 0$, when q is even, one has

$$\begin{aligned}A_q(\mathcal{U}) &= \frac{1}{N} \sum_{k=0}^{q} b(m,k)(-1)^k \\ &= \frac{1}{N} F_m(-1) \\ &= 0.\end{aligned}$$

This completes the proof. □

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