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Optimal designs for order-of-addition experiments

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A B S T R A C T

The order-of-addition (OofA) designs have received significant attention over recent years. It is of great interest to seek for efficient fractional OofA designs especially when the number of components is large. It has been recognized that constructing efficient fractional OofA designs is a challenging work. A systematic construction method for a class of efficient fractional OofA designs, called OofA orthogonal arrays (OofA-OAs), is proposed. It is shown that OofA-OAs are superior over any other type of fractional OofA designs for the predominant pair-wise ordering (PWO) model. The balance property of OofA-OAs is also developed. In addition, the capacity of OofA-OAs for estimating different models is investigated.

1. Introduction

The order-of-addition (OofA) experiment aims at determining the optimal order for processing components in the experiment, which is essential in many areas. For example, in agriculture, Wagner (1995) investigated the order for mixing feed rations and the time spent in blending two types of mixers. The order of addition also matters in chemistry, Fuleki and Francis (1968) stated that “The order of addition of the lead acetate (before or after the pH adjustment) had a definite influence on the reaction. Higher recoveries were obtained by adjusting the pH after lead acetate addition.” The order of addition of reagents is critical in polymerase chain reaction and the sequence of drug administration impacts clinical outcomes (for example, Ding et al., 2015). In genomics, different orders of adding taxa into the computer program yield different likelihoods of the fitted tree (for example, Olsen et al., 1994; Stewart et al., 2001). More applications can be found in Lin and Peng (2019) and references therein.

The study on OofA problem has increasingly aroused the attention of researchers in academe. Van Nostrand (1995) proposed the pair-wise ordering (PWO) model (as will be introduced in Section 2) which assumes that the responses of different orders depend on the pair-wise orders of components. Lin and Peng (2019) highlighted the prospect of the PWO model from many aspects including wide applications, easy utilizations and strong interpretability. Mee (2020) extended the PWO model by taking account of the higher-order interactions between PWO factors. With a different modeling perspective, Yang et al. (2021) developed the component-position (CP) model which assumes that a component has different effects when it is processed at different positions in an order, and Xiao and Xu (2021) proposed the mapping-based universal Kriging model for drug combination experiments.

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Table 1
Full OofA design O_3 and full PWO design P_3.

	PWO factors (P_3)		
O_3	z_{12}	z_{13}	z_{23}
$c_3c_2c_1$	−1	−1	−1
$c_3c_1c_2$	1	−1	−1
$c_2c_3c_1$	−1	−1	1
$c_2c_1c_3$	−1	1	1
$c_1c_3c_2$	1	1	−1
$c_1c_2c_3$	1	1	1

Considering m components, a full OofA design contains $m!$ different orders. In practice, performing an experiment by a full OofA design is usually unaffordable even for a moderately large m (for example, $m = 10$ resulting in $m! \approx 3.6$ millions). It is necessary to choose a subdesign from the full OofA design to perform the experiment. The studies on construction of efficient fractional OofA designs are rather limited in the literature. Voelkel (2019) proposed to use OofA orthogonal arrays (OofA-OAs). As proved in Peng et al. (2019), the OofA-OAs are optimal under a variety of commonly used design criteria including D-, A- and $M.S.$-criteria. Based upon computer search, Voelkel (2019) found a small number of OofA-OAs with 12 or 24 runs for $m = 4, 5, 6$. Peng et al. (2019) provided a closed-form construction method for OofA-OAs in $m!/k!$ runs, where $k = m/2$ for an even m and $k = (m-1)/2$ for an odd m. By employing balanced incompleted block designs, Chen et al. (2020) found some OofA-OAs. The methods in Peng et al. (2019) and Chen et al. (2020) are lack of flexibility in design run size, what's more, the run sizes of their OofA-OAs are quite large. For example when $m = 7$, the run sizes of the OofA-OAs in Peng et al. (2019) and Chen et al. (2020) are 840 and 168, respectively. Yang et al. (2021) and Huang (2021) respectively constructed a class of fractional OofA designs, called component-orthogonal arrays. The component-orthogonal arrays are D-optimal for the CP model but may not be estimable under the PWO model. It is desirable that a fractional OofA design can have good performance for different models. Under the PWO model, Zhao et al. (2021) explored the construction of minimal-point OofA designs, and Winker et al. (2020) generated highly efficient OofA designs via threshold accepting.

In this paper, we propose a systematic construction method for OofA-OAs. Compared to the existing construction methods, the new method enjoys three advantages: (i) it works for any design run size, provided that the OofA-OA exists, (ii) given the run size and the number of components, it is capable of finding many non-equivalent OofA-OAs, and (iii) it is user-friendly due to its elegant mathematical formulation. We address an important unresolved issue in the literature, a D-optimal fractional OofA design is indeed an OofA-OA. It is further proved that any optimal fractional OofA design (in terms of D-, A-, $M.S.$- or χ^2-optimalities) for the PWO model, must be an OofA-OA. The balance property of the OofA-OAs is also investigated. It is shown that the OofA-OAs have a perfect balance property. For example, after removing any $m-3$ components from an OofA-OA, the resulting design has the 6 (3!=6) different orders appearing equally often. It is demonstrated that OofA-OAs can provide considerable relative D-efficiencies (compared to their corresponding full OofA designs) for alternative models (such as CP model).

The rest of the paper is organized as follows. Preliminaries are given in Section 2. The construction method of OofA-OAs is proposed in Section 3. Section 4 explores the balance property of OofA-OAs and proves that, under the PWO model, D-, A-, $M.S.$- or χ^2-optimal fractional OofA designs are OofA-OAs. The performance of OofA-OAs for the CP model is discussed in Section 5. Concluding remarks are given in Section 6. The proofs and some useful design tables are deferred to Appendix.

2. Preliminaries

Denote the m components as $c_1, c_2, \ldots, c_m$. Let O_m denote the *full OofA design* in which the $m!$ rows are $m!$ permutations of the m components. For an order δ in O_m, use $\tau(\delta)$ to represent the expectation of observations arising from order δ. The PWO model is established as

$$\tau(\delta) = \beta_0 + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij}\lambda_{ij}(\delta),$$

where $\lambda_{ij}(\delta) = 1$ if component c_i precedes c_j in δ, otherwise $\lambda_{ij}(\delta) = -1$, and β_0, β_{ij}'s are unknown parameters to be estimated. As an example of $m = 3$, $\lambda_{12}(c_1c_2c_3) = 1$ as c_1 precedes c_2 and $\lambda_{12}(c_2c_3c_1) = -1$ as c_2 precedes c_1. By evaluating all of the $m!$ orders $\delta_1, \delta_2, \ldots, \delta_{m!}$ in O_m, $z_{ij} = (\lambda_{ij}(\delta_1), \lambda_{ij}(\delta_2), \ldots, \lambda_{ij}(\delta_{m!}))^T$ forms an $m!$-dimensional vector relating to the components c_i and c_j. We call z_{ij} a *PWO factor*. For m components, there are in total $m(m-1)/2$ PWO factors z_{ij}'s with $1 \le i < j \le m$. We call the column-juxtaposed matrix $(z_{12}, z_{13}, \ldots, z_{(m-1)m})$ the *full PWO design,* denoted as P_m. As an illustration, the full PWO design P_3 is displayed in Table 1.

For ease of presenting the work, throughout the paper, the rows of O_m are arranged in reversed lexicographical order. For example for $m = 3$, O_3 is displayed in Table 1. The PWO factors in P_m are arranged as $(z_{12}, z_{13}, \ldots, z_{(m-1)m})$, where z_{ij} is ahead of z_{kl} if $i < k$; or if $i = k$ and $j < l$. For example, the PWO factors in P_3 are displayed in Table 1. With such arrangements, each row in P_m is uniquely determined by one row in O_m, and vice versa. We denote D as a fractional OofA design from O_m, and P_D as the corresponding fractional PWO design determined by D.

Definition 1. An N-run fractional OofA design D is called an OofA-OA of strength t, denoted as OofA-OA(N, m, t), if the ratios among the frequencies of all t-tuples in any t-column subarray of P_D equal to the ratios among the frequencies of all t-tuples in the corresponding t-column subarray of P_m.

Definition 1 is a variant of the definition of OofA-OA in Voelkel (2019). In the following, unless particularly stated, the OofA-OAs refer to OofA-OAs of strength $t = 2$. This needs to investigate the frequencies of two-tuples in the two-column subarrays of P_m. Let $n_{(+,+)}$ denote the frequency that the two-tuple $(+, +)$ appears in a pair of PWO factors (columns) of P_m, and $n_{(+,-)}$, $n_{(-,+)}$ and $n_{(-,-)}$ are similarly defined.

Remark 1. Write $d = m(m-1)/2$. For the PWO factors in P_m, the $d(d-1)/2$ pairs (z_{ij}, z_{kl})'s can be classified into three types: the synergistic pairs, satisfying $i = k$ or $j = l$, for which $n_{(+,+)} = m!/3$, $n_{(+,-)} = m!/6$, $n_{(-,+)} = m!/6$ and $n_{(-,-)} = m!/3$; the antagonistic pairs, satisfying $i = l$ or $j = k$, for which $n_{(+,+)} = m!/6$, $n_{(+,-)} = m!/3$, $n_{(-,+)} = m!/3$ and $n_{(-,-)} = m!/6$; and the independent pairs, whose two PWO factors involve no common component, for which $n_{(+,+)} = m!/4$, $n_{(+,-)} = m!/4$, $n_{(-,+)} = m!/4$ and $n_{(-,-)} = m!/4$. Clearly, the run size N of an OofA-OA should be a multiple of 12.

3. Constructions of OofA-OAs

3.1. Constructions of OofA-OA$(N, 4, 2)$'s

To better understand the main idea of the proposed method, we first introduce the idea using $m = 4$ for an illustration in this subsection, and then extend it to a general m in Section 3.2.

Let $b_{ij,kl}(\cdot,\cdot)$ denote the 4!-dimensional vector whose r-th entry is 1, if the two-tuple $(\cdot,\cdot)$ appears in the r-th row of (z_{ij}, z_{kl}) in P_4; and is 0 otherwise. Let

$$B_{ij,kl} = (b_{ij,kl}(+,+), b_{ij,kl}(+,-), b_{ij,kl}(-,+), b_{ij,kl}(-,-)) \text{ and}$$
$$B_{1,2,3,4} = (B_{12,13}, B_{12,14}, \ldots, B_{23,24}),$$

where $B_{ij,kl}$ is ahead of $B_{pq,uv}$ if $i < p$; or if $i = p$ and $j < q$; or if $i = p$, $j = q$ and $k < u$; or if $i = p$, $j = q$, $k = u$ and $l < v$; with $1 \le i, j, k, l, p, q, u, v \le 4$. The matrix $B_{1,2,3,4}$ is displayed in Table B1 in Appendix B. For a fractional OofA design D, if the r-th row δ_r of O_4 is in D, $y_r(D) = 1$, and $y_r(D) = 0$ otherwise. Let $Y_D = (y_1(D), y_2(D), \ldots, y_{4!}(D))^T$. The following theorem establishes a sufficient and necessary condition for a fractional OofA design to be an OofA-OA$(N, 4, 2)$.

Theorem 1. *For $m = 4$, a fractional OofA design D is an OofA-OA$(N, 4, 2)$ if and only if Y_D is a feasible solution of*

$$B^T_{1,2,3,4} Y_D = (N/4!)\text{diag}(B^T_{1,2,3,4} B_{1,2,3,4}), \tag{1}$$

where diag$(\cdot)$ *is a column vector consisting of the diagonal elements of a matrix.*

Theorem 1 indicates that once a feasible solution Y_D of (1) is obtained, we can select an OofA-OA$(N, 4, 2)$ from O_4 according to Y_D. The following example illustrates this point.

Example 1. It is straightforward to verify that $Y_D = (0, 0, 1, 0, 1, 0, 1, 1, 0, 1, 0, 1, 1, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 1)^T$ is a feasible solution of (1), then the OofA design D consisting of the 3, 5, 7, 8, 10, 12, 13, 14, 18, 19, 20, 24-th rows of O_4 is an OofA-OA$(12, 4, 2)$.

By solving (1), there are in total 20 feasible solutions for $N = 12$ and each of them determines an OofA-OA$(12, 4, 2)$. Among these 20 OofA-OA$(12, 4, 2)$'s, 8 of them are isomorphic to $A^{12}_{4.1}$ whose row numbers in O_4 are displayed in Table B2 in Appendix B, and the other 12 are isomorphic to $A^{12}_{4.2}$ in Table B2. Two OofA-OAs are said to be isomorphic if one can be obtained from the other by relabeling components. Throughout the paper, we check isomorphism by relabeling components.

3.2. Constructions of OofA-OA$(N, m, 2)$'s for $m \ge 5$

We now extend the notation Y_D, $b_{ij,kl}(\cdot,\cdot)$ and $B_{ij,kl}$ to a general m. Denote

$$B_{w_1,w_2,w_3,w_4} = (B_{w_1w_2,w_1w_3}, B_{w_1w_2,w_1w_4}, \ldots, B_{w_2w_3,w_3w_4}),$$

where $1 \le w_1 < w_2 < w_3 < w_4 \le m$, $B_{ij,kl}$ is ahead of $B_{pq,uv}$ if $i < p$; or if $i = p$ and $j < q$; or if $i = p$, $j = q$ and $k < u$; or if $i = p$, $j = q$, $k = u$ and $l < v$; with $w_1 \le i, j, k, l, p, q, u, v \le w_4$. Let $B = (B_{1,2,3,4}, B_{1,2,3,5}, \ldots, B_{m-3,m-2,m-1,m})$, where

$B_{i,j,k,l}$ is ahead of $B_{p,q,u,v}$ if $i < p$; or if $i = p$ and $j < q$; or if $i = p$, $j = q$ and $k < u$; or if $i = p$, $j = q$, $k = u$ and $l < v$; with $1 \le i, j, k, l, p, q, u, v \le m$. The theorem below establishes a sufficient and necessary condition for a fractional OofA design to be an OofA-OA$(N, m, 2)$ with a general m.

Theorem 2. *A fractional OofA design D is an OofA-OA*$(N, m, 2)$ *if and only if* Y_D *is a feasible solution of*

$$B^T Y_D = N/(m!)\text{diag}(B^T B). \tag{2}$$

The proof of Theorem 2 is similar to that of Theorem 1 and thus omitted. For $m \ge 5$, it becomes a complex problem to solve (2). To efficiently obtain feasible solutions, we transform (2) into a $0-1$ optimization problem, as stated in Remark 2.

Remark 2. For a given $c \in R^{m!}$, an $m!$-dimensional vector, if Y_D is a feasible solution of the $0-1$ linear optimization problem,

$$\begin{aligned} &\min c^T Y_D \text{ subject to:} \\ &B^T Y_D = N/(m!)\text{diag}(B^T B) \text{ and } Y_D \in \{0,1\}^{m!}, \end{aligned} \tag{3}$$

then Y_D is a feasible solution of equation (2).

Any integer programming solver can be used to solve (3). In this paper, we employ intlinprog in Matlab. For an N and arbitrary c, intlinprog either reports a feasible solution or no feasible solution found (indicating that no OofA-OA exists for such an N). As a sufficient condition, equation (3) may miss some solutions (OofA-OAs) that can be given by equation (2). Note that (2) serves as a sufficient and necessary condition which can provide all possible OofA-OAs.

As an example, we apply Theorem 2 and Remark 2 to seeking for OofA-OAs for $m = 5$, 6, 7. Those designs with small run sizes are displayed in Appendix B.

OofA-OAs for $m = 5$

(i) OofA-OA$(12, 5, 2)$'s. By directly solving equation (2) with $m = 5$ and $N = 12$, there are in total 240 different feasible solutions and each of them provides an OofA-OA$(12, 5, 2)$. Among these OofA-OAs, 120 of them can be obtained from $A_{5.1}^{12}$ in Table B3 in Appendix B by relabeling components, and the other 120 of them can be obtained from $A_{5.2}^{12}$ in Table B3 by relabeling components.

(ii) OofA-OA$(24, 5, 2)$'s. With 2,000 random c's defined in Remark 2, nearly 800 different feasible solutions are found. With these feasible solutions, selective 15 OofA-OA$(24, 5, 2)$'s are displayed in Table B4 in Appendix B. Each of the displayed 15 OofA-OA$(24, 5, 2)$'s cannot be obtained from the others by relabeling components.

(iii) OofA-OA$(36, 5, 2)$'s. With 2,000 random c's defined in Remark 2, nearly 1,200 different feasible solutions are found. With these feasible solutions, selective 15 OofA-OA$(36, 5, 2)$'s are displayed in Table B5 in Appendix B. Each of the displayed 15 OofA-OA$(36, 5, 2)$'s cannot be obtained from the others by relabeling components.

OofA-OAs for $m = 6$

(i) OofA-OA$(12, 6, 2)$ does not exist.

(ii) OofA-OA$(24, 6, 2)$'s. With 2,000 random c's defined in Remark 2, nearly 500 different feasible solutions are found. With these feasible solutions, selective 15 OofA-OA$(24, 6, 2)$'s are displayed in Table B6 in Appendix B. Each of the displayed 15 OofA-OA$(24, 6, 2)$'s cannot be obtained from the others by relabeling components.

(iii) OofA-OA$(36, 6, 2)$'s. With 2,000 random c's defined in Remark 2, nearly 1,000 different feasible solutions are found. With these feasible solutions, selective 15 OofA-OA$(36, 6, 2)$'s are displayed in Table B7 in Appendix B. Each of the displayed 15 OofA-OA$(36, 6, 2)$'s cannot be obtained from the others by relabeling components.

(iv) OofA-OA$(48, 6, 2)$'s. With 2,000 random c's defined in Remark 2, nearly 900 different feasible solutions are found. With these feasible solutions, selective 15 OofA-OA$(48, 6, 2)$'s are displayed in Table B8 in Appendix B. Each of the displayed 15 OofA-OA$(48, 6, 2)$'s cannot be obtained from the others by relabeling components.

OofA-OAs for $m = 7$

(i) OofA-OA$(12, 7, 2)$ does not exist.

(ii) OofA-OA$(24, 7, 2)$'s. With 2,000 random c's defined in Remark 2, nearly 1,100 different feasible solutions are found. With these feasible solutions, selective 15 OofA-OA$(24, 7, 2)$'s are in Table B9 in Appendix B. Each of the displayed 15 OofA-OA$(24, 7, 2)$'s cannot be obtained from the others by relabeling components.

Theorems 1 and 2 imply three salient features of the proposed method. First, the proposed method can provide OofA-OAs for almost any N. Second, given m and N, the proposed method is capable of constructing many non-equivalent OofA-OAs. Different OofA-OAs may have different performances. This will be clearly addressed in Section 5. Third, the proposed method is easy to use due to the simple structure of (2).

4. Theoretical properties of OofA-OAs

4.1. Balance property of OofA-OAs

An example is first provided to illustrate the development in this section.

Example 2. The design

$$A_{4.2}^{12} = \begin{pmatrix} c_4 & c_4 & c_3 & c_3 & c_3 & c_3 & c_2 & c_2 & c_2 & c_1 & c_1 & c_1 \\ c_2 & c_1 & c_4 & c_4 & c_2 & c_1 & c_4 & c_4 & c_1 & c_4 & c_4 & c_2 \\ c_3 & c_3 & c_2 & c_1 & c_1 & c_2 & c_3 & c_1 & c_3 & c_3 & c_2 & c_3 \\ c_1 & c_2 & c_1 & c_2 & c_4 & c_4 & c_1 & c_3 & c_4 & c_2 & c_3 & c_4 \end{pmatrix}^T$$

(displayed in Table B2 in Appendix B) is an OofA-OA$(12, 4, 2)$. Projecting $A_{4.2}^{12}$ onto components c_1 and c_2 results in the design H_1,

$$H_1 = \begin{pmatrix} c_2 & c_1 & c_2 & c_1 & c_2 & c_1 & c_2 & c_2 & c_2 & c_1 & c_1 & c_1 \\ c_1 & c_2 & c_1 & c_2 & c_1 & c_2 & c_1 & c_1 & c_1 & c_2 & c_2 & c_2 \end{pmatrix}^T,$$

which is a 6-replication of O_2. Projecting $A_{4.2}^{12}$ onto components c_1, c_2 and c_3 results in the design H_2,

$$H_2 = \begin{pmatrix} c_2 & c_1 & c_3 & c_3 & c_3 & c_3 & c_2 & c_2 & c_2 & c_1 & c_1 & c_1 \\ c_3 & c_3 & c_2 & c_1 & c_2 & c_1 & c_3 & c_1 & c_1 & c_3 & c_2 & c_2 \\ c_1 & c_2 & c_1 & c_2 & c_1 & c_2 & c_1 & c_3 & c_3 & c_2 & c_3 & c_3 \end{pmatrix}^T,$$

which is a 2-replication of O_3. It is always the case when projecting $A_{4.2}^{12}$ onto other two or three components.

We now formally introduce the balance property of OofA-OAs as indicated in Example 2.

Theorem 3. *For any OofA-OA$(N, m, 2)$ D,*

(i) *when D is projected onto any two components c_i and c_j, the resulting design is an $N/2$-replication of O_2;*
(ii) *when D is projected onto any three components c_i, c_j and c_k, the resulting design is an $N/6$-replication of O_3.*

With the proof of Theorem 3, a sufficient condition for the OofA-OAs is derived.

Corollary 1. *When a fractional OofA design D is projected onto any s components with $s \geq 4$, if all of the $s!$ orders of these s components appear equally often in the resulting design, then D is an OofA-OA.*

Theorem 3 implies that when an OofA-OA is projected onto any two or three components, the resulting designs preserve perfect order balances. As indicated in Example 2, when removing a component from an OofA-OA(12,4,2), all of the 6 orders of the remaining three components appear equally 2 times in the resulting design, and when removing two components from an OofA-OA(12,4,2), all of the 2 orders of the remaining two components appear equally 6 times in the resulting design. Corollary 1 serves as a sufficient condition for seeking for OofA-OAs. It shows that a fractional OofA design is an OofA-OA as long as the $s!$ $(s \geq 4)$ orders of its any s components appear equally after components collapsing.

4.2. Equivalence between the OofA-OA and multi-optimalities

In the literature, it was conjectured that a D-optimal fractional OofA design may be an OofA-OA (Voelkel, 2019). Here, we prove that this is indeed the case. Furthermore, we show that the OofA-OAs are the unique type of fractional OofA designs which possess D-, A-, $M.S.$- and χ^2-optimality.

For an N-run fractional OofA design D, let X be its model matrix under the PWO model, the D-efficiency is defined as $\det(M)^{1/q}$, where $M = X^T X/N$ is the moment matrix of D, q is the number of columns in X and N is the number of rows in X. Peng et al. (2019) proved that a fractional OofA design is optimal with respect to the D-criterion if and only if it has the same moment matrix as the full OofA design. Clearly, OofA-OAs have the same moment matrices as the full OofA designs, and thus are D-optimal. In the following, we show that any D-optimal fractional OofA design must be an OofA-OA. Before formally introducing this result, we first provide a useful lemma. Similar to Theorem 2, the equation for the D-optimal OofA design of N runs can be formulated as in Lemma 1.

Lemma 1. *An N-run fractional OofA design D has the same moment matrix as the full OofA design O_m if and only if, for any two different PWO factors z_{ij} and z_{kl} in P_m, the equations*

$$(z_{ij} \odot Y_D)^T 1_{m!} = 0 \text{ and} \tag{4}$$

$$(z_{ij} \odot Y_D)^T (z_{kl} \odot Y_D) = \begin{cases} N/3, & i = k \text{ and } j \neq l; \text{ or } j = l \text{ and } i \neq k, \\ -N/3, & i = l \text{ and } j \neq k; \text{ or } j = k \text{ and } i \neq l, \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

hold for Y_D, where $1_{m!}$ is an m!-dimensional vector of unity, $1 \le i, j, k, l \le m$ and $\odot$ is the element-wise product.

Combining Lemma 1 with Theorem 3, we have Theorem 4 below.

Theorem 4. *A fractional OofA design is D-optimal if and only if it is an OofA-OA.*

In Peng et al. (2019), some other design criteria such as the A-criterion (defined as trace(M^{-1})) and $M.S.$-criterion (defined as trace(M^2)) are also considered. Under the PWO model, Voelkel (2019) proposed a modified χ^2-criterion to measure the orthogonality of OofA designs. It is defined as

$$\chi^2(D) = \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} \chi^2_{kl}(P_D) / (d\,(d-1)),$$

where $\chi^2_{kl}(P_D) = \sum_{a=\pm 1} \sum_{b=\pm 1} (n_{kl}(a,b) - NE_{kl}(a,b)/m!)^2 / (NE_{kl}(a,b)/m!)$, $n_{kl}(a,b)$ is the number of two-tuple (a,b) which appears in the two-column subarray consisting of the k-th and l-th columns of P_D, and $E_{k,l}(a,b)$ is the number of the two-tuple (a,b) which appears in the two-column subarray consisting of the k-th and l-th columns of the full PWO design P_m. Peng et al. (2019) proved that a fractional OofA design is A- and $M.S.$-optimal if and only if it has the same moment matrix as the full OofA design. From the definitions of OofA-OA and χ^2-criterion, it is evident that a fractional OofA design has the same χ^2-optimality ($\chi^2 = 0$), as the full OofA design if and only if it is OofA-OA. With Theorem 4, we can conclude the result in Corollary 2 below.

Corollary 2. *A fractional OofA design with D-, A-, M.S.- or χ^2-optimality must be an OofA-OA.*

Theorem 4 and Corollary 2 indicate that no fractional OofA design has equal or better performance than the OofA-OAs under the D-, A-, $M.S.$- or χ^2-criterion. This theoretical result strengthens the superiority of OofA-OAs over any other type of fractional OofA designs.

5. Performance of OofA-OAs under an alternative model

Another surrogate model for OofA experiments is the component-position (CP) model (Yang et al., 2021). Denote $\tau_{c_i}^{(j)}$ as the effect of the component c_i at the j-th position of an order involving m components, where $i, j = 1, 2, \ldots, m$. The CP model is established as

$$y = \mu_0 + \sum_{i=1}^{m} \sum_{j=1}^{m} x_{c_i}^{j} \tau_{c_i}^{(j)} + \varepsilon$$

with the baseline constraints

$$\begin{cases} \tau_{c_1}^{(j)} = 0, & \text{for } j = 1, 2, \ldots, m, \\ \tau_{c_i}^{(m)} = 0, & \text{for } i = 1, 2, \ldots, m, \end{cases}$$

where μ_0 is the overall mean, $x_{c_i}^{j} = 1$ if, in order δ, the component c_i is arranged at position j and 0 otherwise, and $\varepsilon \sim N(0, \sigma^2)$ is a random measurement error. It is desirable that a fractional OofA design can be efficient for both the PWO and CP models. Motivated by this, the relative D-efficiencies of the OofA-OAs (compared to their corresponding full OofA designs) for the CP model are investigated, where by converting X and M (see Section 4.2) into their counterparts for the CP model, the D-efficiency for the CP model is also defined as $\det(M)^{1/q}$. We use D_{CP}-efficiency to denote this D-efficiency so as to differentiate it from that for the PWO model. The relative D_{CP}-efficiency of a fractional OofA design is the ratio between the D_{CP}-efficiency of this fractional OofA design and that of its corresponding full OofA design. The CP model has $(m-1)^2 + 1$ parameters to be estimated, an OofA-OA with run size smaller than $(m-1)^2 + 1$ is nonestimable under the CP model.

OofA-OAs for $m = 4$

When $m = 4$, the CP model has 10 parameters to be estimated. From Table B2, $A_{4.1}^{12}$ provides a relative D_{CP}-efficiency 0.76, and $A_{4.2}^{12}$ provides a relative D_{CP}-efficiency 0.

OofA-OAs for $m = 5$

When $m = 5$, the CP model has 17 parameters to be estimated. The OofA-OA(12,5,2)'s are nonestimable under the CP model. The OofA-OA(24,5,2)'s displayed in Table B4 provide relative D_{CP}-efficiencies varying from 0.76 to 0.85. The OofA-OA(36,5,2)'s displayed in Table B5 provide relative D_{CP}-efficiencies varying from 0.88 to 0.90.

OofA-OAs for $m = 6$

When $m = 6$, the CP model has 26 parameters to be estimated. The OofA-OA(24,6,2)'s are nonestimable under the CP model. The OofA-OA(36,6,2)'s displayed in Table B7 provide relative D_{CP}-efficiencies varying from 0.68 to 0.72 and OofA-OA(48,6,2)'s displayed in Table B8 provide relative D_{CP}-efficiencies varying from 0.78 to 0.82.

Relabeling the components of OofA-OAs does not change their relative D_{CP}-efficiencies. While, the OofA-OAs in Tables B2, B4, B5, B7 and B8, have different relative D_{CP}-efficiencies. This implies that non-equivalent OofA-OAs may have different performances under the D_{CP}-criterion. These findings show that the proposed method sheds light on potential wide applications of OofA-OAs beyond the PWO model.

6. Concluding remarks

Constructing efficient fractional OofA designs has been of great interest due to the economical reason. In this paper, we propose a systematic construction method for OofA-OAs, a class of D-, A-, $M.S.$- and χ^2-optimal designs for the predominant PWO model. The proposed construction method has three advantages: (i) it works for any design run size, provided the OofA-OA exists, (ii) given m and N, it is capable of constructing non-equivalent OofA-OAs, and (iii) it is user-friendly due to its elegant mathematical formulation.

The balance property of the OofA-OAs was also investigated. It is shown that, for example, when removing $m - 2$ components from an OofA-OA, all of the 2 $(= 2!)$ orders of the remaining two components appear equally often in the resulting design; and when removing $m - 3$ components from an OofA-OA, all of the 6 $(= 3!)$ orders of the remaining three components appear equally often in the resulting design. Theorem 4 and Corollary 2 show that the OofA-OA is the unique type of fractional OofA designs possessing D-, A-, $M.S.$- and χ^2-optimalities for the PWO model. This theoretical result strengthens the superiority of the OofA-OAs over any other type of fractional OofA designs.

In Section 5, the performances of the OofA-OAs for the CP model are evaluated. OofA-OAs are D-optimal for the PWO model but not necessarily D-optimal for the CP model. Nevertheless, many OofA-OAs can provide considerable relative D-efficiencies (for example, 0.9) for the CP model as indicated in Tables B2, B4, B5, B7 and B8. Similarly, component orthogonal arrays (COAs) proposed in Yang et al. (2021) are D-optimal for the CP model but not necessarily D-optimal for the PWO model. As discussed in Table 5 in Yang et al. (2021), many COAs can provide considerable relative D-efficiencies (for example, 0.9) for the PWO model. This shows that OofA-OAs and COAs are compatible. Xiao and Xu (2021) proposed to use Kriging models (including universal Kriging model and mapping-based universal Kriging model) for the OofA problem. We performed preliminary simulations designed similar to that of Example 2 in Xiao and Xu (2021). It was shown that OofA-OAs have generally good performances evaluated by the criteria used in Xiao and Xu (2021). For example, the tabulated OofA-OA$(N, 6, 2)$'s with $N = 24, 36$ and 48 generally provide R_1 as well as R_2 higher than 0.95 and RMSE ranging from 1 to 3, where R_1 is the correlation between the actual and predicted responses of all observations, R_2 is the correlation between the actual and predicted responses of observations in the test set, and RMSE is the root mean squared error of predicted responses of observations in the test set. A concrete study on the performances of OofA-OAs for the Kriging models will be carried out in our future research.

As pointed by one of the referees, one idea is to minimize the distance between the two sides of the equation (2) instead of making it as a constraint. The linear term in the original objective function in (3) can be either dropped or just added to the previously stated distance measure. In either case, we can use solvers of integer quadratic programming to find the design. It has the same computational complexity as the integer linear programming.

For $m \leq 6$, the integer linear programming can handle any run size provided that the corresponding OofA-OA exists. For $m = 7$, the integer linear programming can only handle some limited run sizes (say $N < 36$). At present, the equation system (2) is too precise to find solutions for large m and N by integer linear programming. One possibility to make the integer linear programming work for $m = 7$ with $N \geq 36$ or $m \geq 8$ is to simplify the equation system (2). To do so, the balance properties developed in Theorem 3 can be useful. As has been previously demonstrated, the newly proposed method is capable of finding D-efficient OofA-OAs under the CP model, systematic study on efficiently finding OofA-OAs with larger D-efficiencies under the CP model is another research direction.

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Appendix A. Proofs

To differentiate the columns in P_m and P_D, in the following proofs, we use x_{ij} to denote the column of P_D corresponding to z_{ij} in P_m.

Proof of Theorem 1. Let $f_{(+,+)}$ be the frequency that the two-tuple $(+,+)$ appears in a pair of PWO factors (columns) of P_D, and $f_{(+,-)}$, $f_{(-,+)}$ and $f_{(-,-)}$ are similarly defined. From Definition 1 and Remark 1, if OofA design D is an OofA-OA of N runs, then $f_{(+,+)} = N/3$, $f_{(+,-)} = N/6$, $f_{(-,+)} = N/6$ and $f_{(-,-)} = N/3$ for any synergistic pair in P_D; $f_{(+,+)} = N/6$, $f_{(+,-)} = N/3$, $f_{(-,+)} = N/3$ and $f_{(-,-)} = N/6$ for any antagonistic pair in P_D; and $f_{(+,+)} = N/4$, $f_{(+,-)} = N/4$, $f_{(-,+)} = N/4$ and $f_{(-,-)} = N/4$ for any independent pair in P_D.

With the definition of $B_{1,2,3,4}$, and some algebra calculations,

$$\text{diag}((N/4!)B_{1,2,3,4}^T B_{1,2,3,4}) = (b_1^T, b_1^T, b_2^T, b_2^T, b_3^T, b_1^T, b_1^T, b_3^T, b_2^T, b_3^T, b_1^T, b_1^T, b_1^T, b_2^T, b_1^T)^T$$

with

$$b_1 = (N/3, N/6, N/6, N/3)^T,$$
$$b_2 = (N/6, N/3, N/3, N/6)^T \text{ and}$$
$$b_3 = (N/4, N/4, N/4, N/4)^T.$$

Note that $b_{ij,kl}(a,b)^T Y_D$ is the frequency of two-tuple (a,b) appearing in (x_{ij}, x_{kl}) of P_D and (1) is a joint of the following equations,

(i) for either $i = k$ or $j = l$, $b_{ij,kl}(a,b)^T Y_D = \begin{cases} N/3, & \text{if } a = + \text{ and } b = +, \\ N/6, & \text{if } a = + \text{ and } b = -, \\ N/6, & \text{if } a = - \text{ and } b = +, \\ N/3, & \text{if } a = - \text{ and } b = -, \end{cases}$

(ii) for either $i = l$ or $j = k$, $b_{ij,kl}(a,b)^T Y_D = \begin{cases} N/6, & \text{if } a = + \text{ and } b = +, \\ N/3, & \text{if } a = + \text{ and } b = -, \\ N/3, & \text{if } a = - \text{ and } b = +, \\ N/6, & \text{if } a = - \text{ and } b = -, \end{cases}$

(iii) for mutually different i, j, k, l, $b_{ij,kl}(a,b)^T Y_D = N/4$ with $a = \pm$ and $b = \pm$.

For proving the "if" part, suppose Y_D is a feasible solution of (1), then (i), (ii) and (iii) are valid. Therefore, P_D has the frequencies of two-tuples required in Definition 1 and thus D is an OofA-OA$(N, 4, 2)$. For proving the "only if" part, if D is an OofA-OA, then P_D has the frequencies of the two-tuples required in Definition 1 implying that (i), (ii) and (iii) hold for Y_D. Therefore, Y_D is a feasible solution of (1). This completes the proof. □

Proof of Theorem 3. We first prove the case of $m = 4$. Applying the Gauss–Jordan elimination to (1), it is obtained that

$$y_1 + y_{24} = N/12, \tag{6}$$
$$y_2 - y_{21} - y_{22} - y_{24} = -N/12, \tag{7}$$
$$y_3 + y_{22} = N/12, \tag{8}$$
$$y_4 - y_{22} - y_{23} - y_{24} = -N/12, \tag{9}$$
$$y_5 + y_{19} + y_{21} + y_{22} = N/6, \tag{10}$$
$$y_6 + y_{20} + y_{23} + y_{24} = N/6, \tag{11}$$
$$y_7 + y_{23} = N/12, \tag{12}$$
$$y_8 - y_{19} - y_{20} - y_{23} = -N/12, \tag{13}$$
$$y_9 + y_{20} = N/12 \tag{14}$$
$$y_{10} - y_{20} - y_{23} - y_{24} = -N/12, \tag{15}$$
$$y_{11} + y_{19} + y_{20} + y_{21} = N/6, \tag{16}$$
$$y_{12} + y_{22} + y_{23} + y_{24} = N/6, \tag{17}$$
$$y_{13} + y_{21} = N/12, \tag{18}$$

$$y_{14} - y_{19} - y_{20} - y_{21} = -N/12, \tag{19}$$

$$y_{15} + y_{19} = N/12, \tag{20}$$

$$y_{16} - y_{19} - y_{21} - y_{22} = -N/12, \tag{21}$$

$$y_{17} + y_{19} + y_{20} + y_{23} = N/6, \text{ and} \tag{22}$$

$$y_{18} + y_{21} + y_{22} + y_{24} = N/6, \tag{23}$$

where (D) is dropped from the notation $y_i(D)$'s for saving space.

For (i). The sum of the left-hand sides of equations (7), (10), (11), (13), (16) and (17) is $y_2 + y_5 + y_6 + y_8 + y_{11} + y_{12} + y_{19} + y_{20} + y_{21} + y_{22} + y_{23} + y_{24}$, and the sum of the right-hand sides of these equations is $N/2$. By checking the orders in O_4, orders with c_1 preceding c_2 appear in $2, 5, 6, 8, 11, 12, 19, 20, 21, 22, 23, 24$-th rows in O_4. This shows that the order c_1c_2 appears $N/2$ times when an OofA-OA$(N, 4, 2)$ is projected onto components c_1 and c_2. Similarly, it can be verified that (i) holds for all of the two orders of any two-component combinations. □

For (ii). The sum of the left-hand sides of equations (7), (13), (16) and (17) is $y_2 + y_8 + y_{11} + y_{12}$, and the sum of the right-hand sides of these equations is $N/6$. By checking the orders in O_4, orders with c_3 preceding c_1 and c_1 preceding c_2 appear in $2, 8, 11, 12$-th rows in O_4. This shows that the order $c_3c_1c_2$ appears $N/6$ times when an OofA-OA$(N, 4, 2)$ is projected onto components c_1, c_2 and c_3. Similarly, it can be verified that (ii) holds for all of the six orders of any three-component combinations.

For $m \geq 5$, the equation (2) is a joint of the $m(m-1)(m-2)(m-3)/24$ equations

$$B^T_{w_i,w_j,w_k,w_l} Y_D = N/(m!)\text{diag}(B^T_{w_i,w_j,w_k,w_l} B_{w_i,w_j,w_k,w_l}) \tag{24}$$

with $1 \leq w_i < w_j < w_k < w_l \leq m$ and B_{w_i,w_j,w_k,w_l} is $m!/4!$-replication of the $B_{1,2,3,4}$ for $m = 4$. Therefore, Theorem 3 holds for $m \geq 5$ as well. □

Proof of Corollary 1. We only need to prove the case of $s = 4$. When D is projected onto any four components $c_{w_i}, c_{w_j}, c_{w_k}$ and c_{w_l}, if all of the 24 orders of $c_{w_i}, c_{w_j}, c_{w_k}, c_{w_l}$ appear equally often in the resulting design, then equation (24) is satisfied. This completes the proof. □

Proof of Lemma 1. The proof of Lemma 1 is similar to that of Theorem 1 by noting that $(z_{ij} \odot Y_D)^T 1_{m!} = x^T_{ij} 1_N$ and $(z_{ij} \odot Y_D)^T (z_{kl} \odot Y_D) = x^T_{ij} x_{kl}$, where 1_N is an N-dimensional vector of unity. We omit the details here. □

Proof of Theorem 4. We first prove Theorem 4 with $m = 4$. Let $h_{ij,kl}$ be a 4!-dimensional vector whose r-th entry is 1 if the two-tuples $(+, +)$ or $(-, -)$ appears in the r-th row of (z_{ij}, z_{kl}) in P_4, and is -1 otherwise, Let

$$H_{1,2,3,4} = (h_{12,13}, h_{12,14}, \ldots, h_{23,24}),$$

where $h_{ij,kl}$ is ahead of $h_{pq,uv}$ if $i < p$; or if $i = p$ and $j < q$; or if $i = p$, $j = q$ and $k < u$; or if $i = p$, $j = q$, $k = u$ and $l < v$; with $1 \leq i, j, k, l, p, q, u, v \leq 4$. Since $(z_{ij} \odot Y_D)^T (z_{kl} \odot Y_D) = (z_{ij} \odot z_{kl})^T Y_D = h^T_{ij,kl} Y_D$ and $(z_{ij} \odot Y_D)^T 1_{m!} = z^T_{ij} Y_D = x^T_{ij} 1_N$, then (4) and (5) with $m = 4$ are equivalent to

$$G^T_{1,2,3,4} Y_D = \begin{pmatrix} 0_6 \\ \xi \end{pmatrix}. \tag{25}$$

where $G_{1,2,3,4} = (P_4, H_{1,2,3,4})$ and ξ is a column vector consisting of the diagonal elements of

$$(N/4!) H^T_{1,2,3,4} H_{1,2,3,4}.$$

Applying the Gauss–Jordan elimination to (25) obtains the same equations as (6)–(23) in the proof of Theorem 3. Therefore, (25) is equivalent to (1) implying that, for $m = 4$, a fractional OofA design has the same moment matrix as the full OofA design if and only if it is an OofA-OA.

With a similar argument to the case of $m = 4$, it is obtained that Theorem 4 holds for $m \geq 5$. This completes the proof. □

Appendix B. Some selective designs

Table B1
Matrix $B^T_{1,2,3,4}$.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
$b^T_{12,13}(+,+)$	1	0	1	0	0	0	1	0	1	0	0	0	1	0	1	0	0	0	1	0	1	0	0	0
$b^T_{12,13}(+,-)$	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0
$b^T_{12,13}(-,+)$	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0
$b^T_{12,13}(-,-)$	0	0	0	1	0	1	0	0	0	1	0	1	0	0	0	1	0	1	0	0	0	1	0	1
$b^T_{12,14}(+,+)$	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0
$b^T_{12,14}(+,-)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	1	0
$b^T_{12,14}(-,+)$	0	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$b^T_{12,14}(-,-)$	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1
$b^T_{12,23}(+,+)$	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0
$b^T_{12,23}(+,-)$	0	0	1	0	1	0	0	0	1	0	1	0	0	0	1	0	1	0	0	0	1	0	1	0
$b^T_{12,23}(-,+)$	0	1	0	1	0	0	0	1	0	1	0	0	0	1	0	1	0	0	0	1	0	1	0	0
$b^T_{12,23}(-,-)$	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1
$b^T_{12,24}(+,+)$	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$b^T_{12,24}(+,-)$	0	0	0	0	0	0	0	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0
$b^T_{12,24}(-,+)$	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0
$b^T_{12,24}(-,-)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	1
$b^T_{12,34}(+,+)$	1	0	1	0	1	0	0	0	1	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0
$b^T_{12,34}(+,-)$	0	0	0	0	0	0	1	0	0	0	0	0	1	0	1	0	0	0	1	0	1	0	1	0
$b^T_{12,34}(-,+)$	0	1	0	1	0	1	0	0	0	1	0	1	0	0	0	0	0	1	0	0	0	0	0	0
$b^T_{12,34}(-,-)$	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	1	0	0	0	1	0	1	0	1
$b^T_{13,14}(+,+)$	1	1	1	0	0	0	1	1	1	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0
$b^T_{13,14}(+,-)$	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	1	0	0	0
$b^T_{13,14}(-,+)$	0	0	0	1	1	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
$b^T_{13,14}(-,-)$	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	1	1	1	0	0	0	1	1	1
$b^T_{13,23}(+,+)$	1	1	0	0	0	0	1	1	0	0	0	0	1	1	0	0	0	0	1	1	0	0	0	0
$b^T_{13,23}(+,-)$	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0
$b^T_{13,23}(-,+)$	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0
$b^T_{13,23}(-,-)$	0	0	0	0	1	1	0	0	0	0	1	1	0	0	0	0	1	1	0	0	0	0	1	1
$b^T_{13,24}(+,+)$	1	1	1	0	0	0	1	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
$b^T_{13,24}(+,-)$	0	0	0	0	0	0	0	0	1	0	0	0	1	0	1	0	0	0	1	1	1	0	0	0
$b^T_{13,24}(-,+)$	0	0	0	1	1	1	0	0	0	1	0	1	0	0	0	1	0	0	0	0	0	0	0	0
$b^T_{13,24}(-,-)$	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	1	0	0	0	1	1	1
$b^T_{13,34}(+,+)$	1	1	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$b^T_{13,34}(+,-)$	0	0	0	0	0	0	1	1	0	0	0	0	1	1	1	0	0	0	1	1	1	0	0	0
$b^T_{13,34}(-,+)$	0	0	0	1	1	1	0	0	0	1	1	1	0	0	0	0	1	1	0	0	0	0	0	0
$b^T_{13,34}(-,-)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	1	1
$b^T_{14,23}(+,+)$	1	1	0	1	0	0	1	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
$b^T_{14,23}(+,-)$	0	0	1	0	1	1	0	0	1	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0
$b^T_{14,23}(-,+)$	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	1	0	0	1	1	0	1	0	0
$b^T_{14,23}(-,-)$	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	0	0	1	0	1	1
$b^T_{14,24}(+,+)$	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$b^T_{14,24}(+,-)$	0	0	0	0	0	0	0	0	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0
$b^T_{14,24}(-,+)$	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0
$b^T_{14,24}(-,-)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1
$b^T_{14,34}(+,+)$	1	1	1	1	1	1	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
$b^T_{14,34}(+,-)$	0	0	0	0	0	0	1	1	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0
$b^T_{14,34}(-,+)$	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	1	1	0	0	0	0	0	0
$b^T_{14,34}(-,-)$	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	1	1	1	1	1	1
$b^T_{23,24}(+,+)$	1	1	0	1	0	0	1	1	0	1	0	0	0	1	0	1	0	0	0	0	0	0	0	0
$b^T_{23,24}(+,-)$	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	1	0	1	0	0
$b^T_{23,24}(-,+)$	0	0	1	0	1	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
$b^T_{23,24}(-,-)$	0	0	0	0	0	0	0	0	1	0	1	0	0	0	1	0	1	1	0	0	1	0	1	1
$b^T_{23,34}(+,+)$	1	1	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$b^T_{23,34}(+,-)$	0	0	0	0	0	0	1	1	0	0	0	0	1	1	0	1	0	0	1	1	0	1	0	0
$b^T_{23,34}(-,+)$	0	0	1	0	1	1	0	0	1	0	1	1	0	0	0	0	1	1	0	0	0	0	0	0
$b^T_{23,34}(-,-)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	1	1
$b^T_{24,34}(+,+)$	1	1	1	1	1	1	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0
$b^T_{24,34}(+,-)$	0	0	0	0	0	0	1	1	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0
$b^T_{24,34}(-,+)$	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	1	1	0	0	0	0	0	0
$b^T_{24,34}(-,-)$	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	1	1	1	1	1	1

Table B2
Two OofA-OA(12,4,2)'s.

Run	1	2	3	4	5	6	7	8	9	10	11	12	D_{CP}
$A^{12}_{4.1}$	1	3	6	8	9	12	14	16	18	19	21	23	0.76
$A^{12}_{4.2}$	1	2	4	6	9	11	15	16	17	21	22	23	0

D_{CP}: the relative D_{CP}-efficiency compared to the full OofA design.

Table B3
Two OofA-OA(12,5,2)'s.

Run	1	2	3	4	5	6	7	8	9	10	11	12	D_{CP}
$A^{12}_{5.1}$	1	6	12	18	57	59	81	83	89	05	107	113	*
$A^{12}_{5.2}$	2	15	21	31	48	58	72	80	86	91	104	110	*

* the run size of the OofA-OA is smaller than the number of parameters in the CP model.

Table B4
Selective 15 OofA-OA(24,5,2)'s.

Run	$A^{24}_{5.1}$	$A^{24}_{5.2}$	$A^{24}_{5.3}$	$A^{24}_{5.4}$	$A^{24}_{5.5}$	$A^{24}_{5.6}$	$A^{24}_{5.7}$	$A^{24}_{5.8}$	$A^{24}_{5.9}$	$A^{24}_{5.10}$	$A^{24}_{5.11}$	$A^{24}_{5.12}$	$A^{24}_{5.13}$	$A^{24}_{5.14}$	$A^{24}_{5.15}$
1	3	3	3	3	2	3	3	4	10	2	2	5	5	3	3
2	8	8	5	5	3	8	10	7	13	7	13	15	10	10	8
3	9	18	7	10	9	18	11	22	20	15	15	20	15	12	9
4	18	20	17	14	11	23	14	26	24	17	20	24	17	13	18
5	23	21	22	21	24	25	23	27	27	22	22	26	20	20	23
6	30	25	26	26	28	28	26	30	29	30	25	28	30	21	30
7	33	31	28	36	29	33	36	33	31	33	34	31	33	30	31
8	38	41	35	39	31	45	38	36	36	38	38	41	35	33	33
9	42	45	48	41	41	48	41	48	41	42	45	48	40	36	41
10	45	48	54	49	48	54	43	51	50	45	48	52	43	41	48
11	52	54	57	54	60	56	50	54	57	51	53	57	54	43	53
12	53	59	64	59	61	62	55	64	59	53	55	59	55	49	59
13	59	61	65	64	66	64	61	67	62	60	60	61	57	59	63
14	63	65	69	65	69	67	65	75	72	66	62	67	67	61	71
15	70	70	73	76	78	74	77	77	74	69	72	70	72	70	74
16	73	73	84	80	81	75	82	84	75	79	74	73	73	80	76
17	82	80	86	87	86	82	87	86	84	82	87	76	75	87	82
18	90	87	87	94	88	90	90	90	89	86	89	82	84	90	90
19	92	90	93	101	91	95	102	93	96	92	92	93	93	92	95
20	97	95	102	104	101	97	105	97	97	97	94	95	95	94	97
21	103	100	106	106	106	100	108	101	100	104	99	97	99	105	103
22	113	101	107	111	109	107	109	111	107	114	104	100	107	110	110
23	117	106	109	116	110	112	114	112	109	115	110	114	113	115	112
24	119	117	116	119	117	117	116	116	118	119	117	118	120	119	117
D_{CP}	0.85	0.81	0.80	0.79	0.78	0.78	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.76

D_{CP}: the relative D_{CP}-efficiency compared to the full OofA design.

Table B5
Selective 15 OofA-OA(36,5,2)'s.

	$A^{36}_{5.1}$	$A^{36}_{5.2}$	$A^{36}_{5.3}$	$A^{36}_{5.4}$	$A^{36}_{5.5}$	$A^{36}_{5.6}$	$A^{36}_{5.7}$	$A^{36}_{5.8}$	$A^{36}_{5.9}$	$A^{36}_{5.10}$	$A^{36}_{5.11}$	$A^{36}_{5.12}$	$A^{36}_{5.13}$	$A^{36}_{5.14}$	$A^{36}_{5.15}$
1	6	6	3	3	2	3	3	2	3	2	2	2	3	3	3
2	7	7	4	7	4	5	4	6	5	3	9	3	8	10	6
3	13	8	8	10	10	7	11	11	12	9	11	9	11	11	9
4	16	15	9	15	13	10	12	12	14	11	14	10	12	18	11
5	19	17	11	17	16	12	13	14	15	17	15	11	15	19	14
6	21	22	18	22	21	14	16	15	21	18	19	14	17	23	18
7	24	23	19	23	23	17	19	17	23	19	23	20	23	26	19
8	26	26	23	26	26	21	22	27	25	24	27	22	29	28	21
9	28	27	30	30	29	27	25	29	26	25	30	23	30	31	25

(*continued on next page*)

Table B5 (*continued*)

	$A^{36}_{5.1}$	$A^{36}_{5.2}$	$A^{36}_{5.3}$	$A^{36}_{5.4}$	$A^{36}_{5.5}$	$A^{36}_{5.6}$	$A^{36}_{5.7}$	$A^{36}_{5.8}$	$A^{36}_{5.9}$	$A^{36}_{5.10}$	$A^{36}_{5.11}$	$A^{36}_{5.12}$	$A^{36}_{5.13}$	$A^{36}_{5.14}$	$A^{36}_{5.15}$
10	31	31	32	33	34	32	30	32	34	35	34	31	33	34	27
11	35	33	34	35	37	34	34	33	36	38	38	36	35	38	34
12	39	38	38	38	39	36	36	40	38	39	39	38	36	40	39
13	41	41	40	41	41	38	38	41	39	44	41	41	38	43	42
14	46	45	43	45	44	44	43	43	47	45	45	43	41	45	43
15	48	46	48	46	50	45	47	46	48	48	46	45	45	50	47
16	51	48	52	50	51	53	50	49	49	49	50	47	49	51	50
17	53	51	55	53	55	56	55	52	51	54	52	49	52	56	54
18	58	53	59	55	60	58	59	57	56	56	55	56	55	60	59
19	59	62	61	62	62	63	61	64	62	58	60	57	62	62	60
20	62	64	63	64	64	65	63	65	64	63	62	65	64	66	61
21	63	69	68	70	69	68	65	67	67	65	63	67	70	68	63
22	70	70	70	71	71	74	70	72	71	72	69	72	73	73	65
23	71	71	73	73	74	79	77	75	76	74	72	77	74	74	68
24	73	73	76	74	78	85	81	77	77	79	73	79	82	75	76
25	75	78	81	82	84	86	83	78	83	83	78	82	87	83	80
26	80	82	83	87	87	88	85	82	87	85	82	85	90	87	81
27	90	87	90	90	89	94	90	87	90	89	89	87	92	90	90
28	91	89	93	94	93	96	92	93	92	90	93	90	93	95	92
29	94	91	95	95	98	98	96	99	94	94	95	92	98	98	95
30	95	96	101	98	100	100	101	104	99	99	98	94	100	99	101
31	98	98	103	100	105	106	105	108	101	101	100	102	103	102	105
32	100	100	106	103	106	107	108	110	104	106	103	104	108	108	106
33	103	103	109	107	109	111	109	111	105	107	109	106	109	112	111
34	110	109	113	109	116	116	110	115	111	111	116	111	113	113	115
35	117	117	116	116	118	117	116	119	114	113	118	113	119	117	117
36	120	120	120	120	120	119	118	120	119	116	120	119	120	118	120
D_{CP}	0.90	0.89	0.89	0.89	0.89	0.88	0.88	0.88	0.88	0.88	0.88	0.88	0.88	0.88	0.88

D_{CP}: the relative D_{CP}-efficiency compared to the full OofA design.

Table B6
Selective 15 OofA-OA(24,6,2)'s.

Run	$A^{24}_{6.1}$	$A^{24}_{6.2}$	$A^{24}_{6.3}$	$A^{24}_{6.4}$	$A^{24}_{6.5}$	$A^{24}_{6.6}$	$A^{24}_{6.7}$	$A^{24}_{6.8}$	$A^{24}_{6.9}$	$A^{24}_{6.10}$	$A^{24}_{6.11}$	$A^{24}_{6.12}$	$A^{24}_{6.13}$	$A^{24}_{6.14}$	$A^{24}_{6.15}$
1	1	1	1	3	15	31	56	4	25	22	70	16	4	12	44
2	6	18	15	18	30	95	83	46	46	25	78	58	25	58	85
3	54	29	46	45	67	130	108	65	92	118	81	108	46	85	141
4	112	69	93	69	114	160	160	143	146	124	102	110	53	118	180
5	136	113	119	161	121	170	174	156	162	128	105	133	92	122	199
6	177	133	148	187	137	194	200	171	190	210	127	149	117	138	216
7	216	192	173	263	191	225	223	219	222	255	185	229	146	158	218
8	258	227	227	265	231	252	251	248	255	288	225	273	183	165	253
9	272	263	266	286	308	270	253	267	260	311	227	284	222	209	262
10	283	321	330	325	317	314	288	330	285	339	279	308	233	271	271
11	328	352	348	375	321	337	350	341	330	365	292	315	322	325	300
12	347	395	397	392	352	373	364	379	381	399	332	361	347	338	335
13	376	415	404	408	376	381	385	400	388	412	337	384	415	379	379
14	442	425	421	425	392	408	422	423	399	443	358	407	428	420	387
15	463	440	428	437	418	426	448	462	449	464	362	430	453	444	426
16	473	462	454	507	434	484	475	484	461	499	399	444	458	446	434
17	509	532	498	509	515	542	486	526	485	516	419	488	498	488	462
18	532	539	527	546	531	568	505	533	495	535	478	519	525	546	488
19	555	553	539	600	576	592	576	555	517	556	506	551	541	577	498
20	579	584	541	612	595	606	580	580	591	582	529	583	548	651	583
21	620	593	615	617	612	612	606	644	613	620	571	600	559	669	604
22	661	612	642	633	646	682	627	658	643	635	600	636	636	676	651
23	683	633	661	647	649	692	658	685	690	657	629	649	663	683	706
24	706	647	697	709	704	703	718	718	713	690	692	698	689	708	720
D_{CP}	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*

* the run size of the OofA-OA is smaller than the number of parameters in the CP model.

Table B7
Selective 15 OofA-OA(36,6,2)'s.

	$A^{36}_{6.1}$	$A^{36}_{6.2}$	$A^{36}_{6.3}$	$A^{36}_{6.4}$	$A^{36}_{6.5}$	$A^{36}_{6.6}$	$A^{36}_{6.7}$	$A^{36}_{6.8}$	$A^{36}_{6.9}$	$A^{36}_{6.10}$	$A^{36}_{6.11}$	$A^{36}_{6.12}$	$A^{36}_{6.13}$	$A^{36}_{6.14}$	$A^{36}_{6.15}$
1	7	11	16	23	29	11	16	27	22	8	2	22	49	16	43
2	14	24	26	37	51	25	21	42	25	27	6	65	60	19	49
3	28	41	34	43	78	64	32	43	49	71	59	74	73	44	71
4	90	57	68	53	82	65	66	53	59	90	63	98	94	57	81
5	117	81	83	56	109	104	74	66	75	106	77	118	96	67	96
6	141	91	94	88	132	108	101	74	107	121	84	128	116	74	98
7	146	105	141	95	145	138	121	119	120	126	158	182	139	129	122
8	188	125	152	96	167	149	160	129	133	138	174	216	171	143	164
9	199	154	183	176	170	164	174	159	152	182	198	223	188	159	192
10	240	157	197	203	209	201	226	174	177	190	208	228	196	161	197
11	264	200	203	207	214	255	236	177	197	200	231	243	203	192	207
12	276	215	253	221	267	281	252	211	216	230	263	265	236	236	225
13	291	224	264	230	290	285	268	225	224	237	267	299	244	252	229
14	302	272	284	265	313	308	283	235	258	263	274	305	251	298	267
15	323	282	298	282	326	330	317	249	288	291	286	318	273	299	289
16	328	307	315	291	342	361	327	270	293	310	302	320	290	321	305
17	343	342	347	293	346	390	338	303	322	323	328	341	319	341	331
18	372	353	361	314	367	402	371	311	353	335	364	346	324	346	360
19	388	374	386	340	383	407	399	349	374	363	381	363	343	378	368
20	397	407	404	360	406	413	400	357	407	410	395	382	360	392	377
21	410	413	426	394	426	423	411	380	419	423	412	385	368	409	400
22	455	415	445	398	443	430	431	400	423	429	439	396	405	439	414
23	463	441	480	439	449	482	452	419	456	450	478	413	425	475	423
24	484	456	510	452	479	492	465	460	478	489	508	479	437	496	472
25	496	463	516	457	499	517	492	486	506	514	531	481	444	502	486
26	509	487	521	480	504	521	494	520	531	533	550	495	482	521	487
27	550	496	556	499	516	529	517	532	549	557	571	521	546	530	512
28	562	520	574	505	536	588	538	555	551	564	578	543	561	545	521
29	588	557	603	522	559	593	584	573	558	578	616	550	572	585	550
30	602	590	617	545	606	606	593	592	571	613	625	574	602	598	573
31	617	604	636	631	610	625	612	599	610	621	629	582	610	612	606
32	636	628	657	637	611	634	658	603	635	633	651	609	636	637	618
33	651	669	665	659	639	678	677	632	638	651	672	630	639	655	655
34	688	689	685	672	643	689	679	688	649	660	684	643	683	674	668
35	691	712	697	695	663	701	705	693	679	692	709	676	695	689	683
36	700	717	716	698	720	711	720	709	698	717	716	694	709	720	713
D_{CP}	0.72	0.71	0.70	0.69	0.69	0.69	0.69	0.69	0.68	0.68	0.68	0.68	0.68	0.68	0.68

D_{CP}: the relative D_{CP}-efficiency compared to the full OofA design.

Table B8
Selective 15 OofA-OA(48,6,2)'s.

Run	$A^{48}_{6.1}$	$A^{48}_{6.2}$	$A^{48}_{6.3}$	$A^{48}_{6.4}$	$A^{48}_{6.5}$	$A^{48}_{6.6}$	$A^{36}_{6.7}$	$A^{48}_{6.8}$	$A^{48}_{6.9}$	$A^{48}_{6.10}$	$A^{48}_{6.11}$	$A^{48}_{6.12}$	$A^{48}_{6.13}$	$A^{48}_{6.14}$	$A^{48}_{6.15}$
1	3	8	13	23	8	25	3	27	16	32	7	2	2	5	6
2	16	23	19	33	45	52	5	41	21	57	32	13	24	11	37
3	45	33	35	44	48	53	20	78	28	66	83	63	35	15	52
4	64	69	60	47	55	58	23	86	32	86	84	70	38	37	65
5	70	84	69	54	62	74	36	105	63	97	99	83	55	40	70
6	77	85	75	89	73	89	38	106	101	102	104	100	62	45	84
7	102	92	83	90	82	107	63	115	107	113	110	104	102	61	87
8	105	105	96	133	95	114	90	122	113	133	136	119	120	63	100
9	124	141	125	141	100	124	110	162	145	139	140	157	129	111	121
10	131	152	150	182	144	138	131	176	154	145	164	163	139	120	125
11	133	167	177	190	155	190	136	196	168	154	165	166	159	138	144
12	167	169	178	195	157	201	145	200	170	161	174	189	169	177	188
13	183	202	183	204	175	230	191	218	188	170	208	197	204	188	199
14	188	209	198	224	195	235	207	226	197	190	213	216	210	195	204
15	198	215	218	241	204	246	215	239	207	198	228	219	221	201	206

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Table B8 (*continued*)

Run	$A^{48}_{6.1}$	$A^{48}_{6.2}$	$A^{48}_{6.3}$	$A^{48}_{6.4}$	$A^{48}_{6.5}$	$A^{48}_{6.6}$	$A^{36}_{6.7}$	$A^{48}_{6.8}$	$A^{48}_{6.9}$	$A^{48}_{6.10}$	$A^{48}_{6.11}$	$A^{48}_{6.12}$	$A^{48}_{6.13}$	$A^{48}_{6.14}$	$A^{48}_{6.15}$
16	229	220	220	244	211	260	269	242	237	204	233	239	227	224	232
17	245	226	238	252	222	266	281	247	255	230	241	246	232	234	241
18	250	247	249	283	230	274	298	274	264	267	252	264	241	235	264
19	274	254	267	292	248	281	307	308	292	270	283	265	258	263	281
20	284	260	280	297	257	291	321	321	299	290	291	290	259	271	290
21	290	277	292	310	272	327	344	342	333	314	310	329	321	282	312
22	309	309	325	333	282	332	360	356	337	326	318	331	332	291	320
23	325	321	332	356	295	340	371	366	374	341	320	354	351	296	329
24	331	335	352	362	314	353	375	371	385	342	330	367	357	300	337
25	358	337	358	369	354	362	377	375	406	354	348	374	382	314	385
26	372	354	368	394	357	371	393	387	413	363	369	377	388	343	405
27	408	364	383	416	381	399	395	391	417	370	388	385	395	359	407
28	411	383	388	446	406	403	408	396	431	408	399	417	420	380	413
29	418	399	395	457	424	429	422	422	438	430	413	422	428	394	421
30	433	419	443	476	438	437	443	443	475	445	418	429	441	432	430
31	443	425	448	482	439	447	473	451	482	450	453	467	455	437	436
32	466	436	468	503	449	462	490	480	490	459	457	468	457	452	442
33	511	444	476	509	460	483	502	492	507	478	470	476	480	469	485
34	536	470	488	514	468	501	512	497	528	487	480	493	489	474	520
35	558	476	503	519	485	505	514	507	535	492	481	509	503	509	537
36	559	488	518	521	518	520	547	530	540	519	494	517	511	532	557
37	569	497	531	568	541	528	565	539	551	527	507	535	540	550	582
38	579	505	552	580	569	546	581	546	573	557	513	538	542	560	588
39	594	567	573	599	573	575	586	575	575	563	555	552	555	562	594
40	598	585	577	604	591	596	638	586	581	589	579	564	573	585	608
41	617	591	606	628	601	605	649	603	611	594	588	578	579	590	632
42	634	621	649	633	636	631	654	604	615	613	593	590	584	596	637
43	639	626	657	660	654	633	658	628	630	619	623	609	619	602	662
44	654	642	669	667	655	640	679	646	631	644	624	612	641	625	664
45	674	671	673	678	673	672	686	656	658	657	625	630	656	677	678
46	697	679	686	679	694	683	698	687	672	672	690	633	662	681	697
47	702	701	705	694	699	704	704	690	680	685	691	670	664	707	701
48	712	720	719	714	719	710	714	716	696	699	709	695	691	709	711
D_{CP}	0.82	0.80	0.80	0.80	0.80	0.79	0.79	0.78	0.78	0.78	0.78	0.78	0.78	0.78	0.78

D_{CP}: the relative D_{CP}-efficiency compared to the full OofA design.

Table B9
Selective 15 OofA-OA(24,7,2)'s.

Run	$A^{24}_{7.1}$	$A^{24}_{7.2}$	$A^{24}_{7.3}$	$A^{24}_{7.4}$	$A^{24}_{7.5}$	$A^{24}_{7.6}$	$A^{24}_{7.7}$	$A^{24}_{7.8}$	$A^{24}_{7.9}$	$A^{24}_{7.10}$	$A^{24}_{7.11}$	$A^{24}_{7.12}$	$A^{24}_{7.13}$	$A^{24}_{7.14}$	$A^{24}_{7.15}$
1	5	290	669	56	214	14	117	11	361	230	44	11	83	30	387
2	777	467	783	282	337	449	199	286	671	289	392	148	361	145	524
3	836	482	870	378	416	741	404	387	780	481	588	489	634	469	749
4	928	522	1042	711	483	1452	581	504	999	810	975	664	654	563	787
5	1408	902	1323	891	693	1563	851	821	1086	1113	1104	707	890	835	1053
6	1492	1092	1474	1271	1010	1751	1060	1030	1359	1271	1425	778	1570	1050	1279
7	1900	1350	1637	1589	1160	2016	1240	1696	1506	1323	1539	1066	1720	1124	1433
8	1945	1387	2016	1962	1375	2278	1403	2088	1574	1460	1624	1639	2064	1165	1749
9	2099	1538	2131	1972	1417	2342	1593	2260	1794	1784	1761	1732	2380	1501	1764
10	2236	1642	2192	2125	1563	2387	2102	2321	2192	1999	2061	2021	2474	1797	1805
11	2424	1760	2350	2295	1754	2505	2428	2431	2344	2015	2158	2078	2512	1846	1942
12	2545	1871	2742	2460	1914	2979	2515	2715	2501	2230	2364	2704	2630	2033	2163
13	2568	2170	2897	2621	2113	3064	2625	3080	2538	2436	2409	2774	2910	2428	2279
14	2740	2503	2915	2685	2612	3101	2654	3222	3547	2750	2856	3080	3114	2542	2598
15	2817	2734	3291	3019	2878	3171	2887	3284	3644	2948	2953	3098	3256	2601	2966
16	2983	3049	3592	3318	3040	3771	2952	3467	3653	3118	3038	3192	3461	2774	3311
17	3422	3419	3614	3429	3268	3832	3439	3756	3830	3255	3345	3290	3729	3623	3396
18	3587	3670	3900	3605	3534	3862	3479	3867	3923	3429	3571	3476	3766	3916	4015
19	3709	4165	3979	4131	4012	4095	3852	4097	4141	3705	3658	3838	3892	4163	4184
20	3886	4206	4108	4404	4020	4208	4139	4209	4173	3992	3822	3986	4160	4227	4372
21	4095	4742	4433	4538	4086	4384	4227	4452	4352	4497	3980	4097	4311	4479	4482
22	4305	4809	4501	4562	4230	4686	4359	4633	4545	4797	4189	4511	4490	4818	4579
23	4342	4846	4566	4720	4608	4860	4678	4866	4806	4854	4441	4712	4524	4859	4887
24	4404	5003	4884	5028	4686	4965	4727	5006	4888	4926	4755	4971	4928	5005	4932
D_{CP}	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*

* the run size of the OofA-OA is smaller than the number of parameters in the CP model.

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