Journal of the American Statistical Association

ISSN: 0162-1459 (Print) 1537-274X (Online) Journal homepage: www.tandfonline.com/journals/uasa20

Universally Optimal Designs for Symmetric Models in Order-of-Addition Experiments

Ze Liu, Yongdao Zhou & Min-Qian Liu

To cite this article: Ze Liu, Yongdao Zhou & Min-Qian Liu (30 Oct 2025): Universally Optimal Designs for Symmetric Models in Order-of-Addition Experiments, Journal of the American Statistical Association, DOI: 10.1080/01621459.2025.2552515

To link to this article: https://doi.org/10.1080/01621459.2025.2552515

JOURNAL OF THE AMERICAN STATISTICAL ASSOCIATION
2025, VOL. 00, NO. 0, 1–11: Theory and Methods
https://doi.org/10.1080/01621459.2025.2552515

Universally Optimal Designs for Symmetric Models in Order-of-Addition Experiments

Ze Liu, Yongdao Zhou, and Min-Qian Liu

NITFID, LPMC & KLMDASR, School of Statistics and Data Science, Nankai University, Tianjin, China

ABSTRACT

Recently, a lot of models for order-of-addition (OofA) experiments have been proposed, as well as the corresponding designs. However, most of those researches are under specific models and/or specific criteria, and a general framework is lacked. In this article, we propose a general form of linear models for OofA experiments, called the symmetric linear models. We show that almost all popularly-used linear models for OofA experiments are equivalent to symmetric linear models, and we further prove that the component orthogonal arrays (COAs) of particular strengths are the corresponding universally optimal OofA designs. Conversely, under some particular cases, the optimal OofA designs must be COAs. Furthermore, we propose a systematic method for constructing COAs of strength 3, and provide some specific constructions of COAs of strengths 2, 4 and higher. Numerical results show that COAs perform well under various criteria. Supplementary materials for this article are available online, including a standardized description of the materials available for reproducing the work.

ARTICLE HISTORY
Received November 2023
Accepted August 2025

KEYWORDS
Component orthogonal array; Component-position model; Pairwise ordering model; Symmetric linear model; Universal optimality

1. Introduction

In an order-of-addition (OofA) experiment, the interest is to investigate whether and how the order in which several different components are added can affect the response. An early example of OofA experiments is the famous story of "a lady tasting tea" (Fisher 1971, chap. II). The OofA experiments are becoming more and more important in both scientific and industrial researches, having applications in many areas including chemistry, food science, drug combination study, job scheduling, etc.; please refer to Lin and Peng (2019), Huang (2021), Zhao, Lin, and Liu (2022) and the references therein for details. The idea of OofA experiments can even be used in numerical approximation (Yang et al. 2024). With m components, the number of all possible orders $m!$ is very large even for a moderate m, and we can only observe the responses corresponding to a small number of orders. Therefore, appropriate model assumptions and experimental designs play important roles in planning OofA experiments. Van Nostrand (1995) first proposed the pairwise ordering (PWO) model for OofA experiments. Lin and Peng (2019) gave a review of OofA experiments. As pointed out by Mee (2024), the statistical literature on OofA experiments has explosively increased recently, with many new models being proposed, as well as the corresponding experimental designs. Researches on experiments involving both OofA effects and other kinds of effects also begin to emerge recently, see for example, Rios, Winker, and Lin (2022), Yang, Zhou, and Liu (2023), and Xiao et al. (2024). In this article, we will propose a general class of linear models for OofA experiments, derive the corresponding optimal designs, and provide construction methods for some of the optimal designs.

With an assumed model, a common task is to find optimal designs under various information-based criteria, for example, the D-, A-, and E-criteria. For example, Peng, Mukerjee, and Lin (2019) proved that the OofA orthogonal arrays (OofA-OAs) of strength 2 proposed by Voelkel (2019) are the only designs with optimal design measures for the PWO model under a broad class of optimality criteria (also refer to Zhao, Lin, and Liu 2022). Other linear models based on the relative positions of components have been proposed by Lin and Peng (2019), Peng, Mukerjee, and Lin (2019), Mee (2020), and Chen et al. (2023), among others, but there is still no result on the corresponding optimal fractional designs. On the other hand, based on the absolute positions of components, Yang, Sun, and Xu (2021) proposed the component-position (CP) model, along with a new type of OofA designs called the component orthogonal array (COA) which is D-optimal under their CP model. Successively, Stokes and Xu (2022) proposed a broad class of polynomial models and obtained the D-optimality of COAs under their polynomial models without interactions, but did not provide the corresponding D-optimal fractional designs for their models involving interactions. Furthermore, Zhao, Li, and Zhao (2021) generalized the definition of COAs and proved that COAs of strength 4 are D-optimal for the PWO model. However, most of the above researches are under specific models and/or specific criteria, and some of them involve cumbersome calculations. An exception is Peng, Mukerjee, and Lin (2019), which inspires us to establish a unified framework in this article. Precisely, almost all popularly-used linear models for OofA experiments are equivalent to symmetric linear models which will be defined in this article. Moreover, we will prove that COAs of particular strengths are the only type of designs having universally optimal

CONTACT Min-Qian Liu *mqliu@nankai.edu.cn* NITFID, LPMC & KLMDASR, School of Statistics and Data Science, Nankai University, Tianjin 300071, China.
Supplementary materials for this article are available online. Please go to *www.tandfonline.com/r/JASA*.

design measures under all symmetric linear models simultaneously. These will cover many existing results.

Another important issue is the systematic construction of designs. Peng, Mukerjee, and Lin (2019) gave a systematic construction method for OofA-OAs of strength 2 with any numbers of components, and Chen, Mukerjee, and Lin (2020) improved their method. As for COAs of strength 2, Yang, Sun, and Xu (2021) proposed a systematic construction method for prime-power numbers of components, starting from which Huang (2021) developed a method to construct COAs of strength 2 for any numbers of components by recursively adding components. In this article, we generalize this recursive construction method to a more flexible one which applies to COAs of general strengths, and use it to provide some particular COAs of strength 2. As for COAs of strength 3, the only available results are provided by Zhao, Li, and Zhao (2021) through solving 0–1 linear programming problems, which is not applicable when the number of components is greater than 6. In comparison, we propose a systematic construction method for COAs of strength 3 and index 1 which is applicable for any number of components being a prime power plus one. Additionally, we investigate the construction of COAs with higher strengths and some new results are obtained.

The rest of this article is organized as follows. Section 2 proposes a general form of linear models for OofA experiments, called the symmetric linear models, and justifies how the popularly-used linear models are included as special cases in the sense of equivalence. In Section 3, we introduce the definition of COAs, and study the universal optimality of COAs under symmetric models. Section 4 proposes two augmentation methods for COAs of general strengths and a construction method for COAs of strength 3, and discusses the construction of COAs with higher strengths. Finally, some concluding remarks are provided in Section 5. To save space, additional examples and theories, numerical comparisons, and the proofs of the main theoretical results are all deferred to the supplementary materials.

2. Symmetric Linear Models

First, we introduce some basic notations. Let $\mathbb{N}$ be the set of natural numbers, $\mathbb{N}_+$ be the set of positive integers and $\mathbb{R}$ be the set of real numbers. For any $k \in \mathbb{N}$, let $\mathcal{Z}_k = \{0, 1, \ldots, k-1\}$ be the set of the first k natural numbers, let $\mathcal{Z}_k^{N\times l}$ be the set of $N \times l$ matrices whose entries are in $\mathcal{Z}_k$, and denote $\mathcal{Z}_k^{1\times l}$ by $\mathcal{Z}_k^l$. For convenience, the indices of entries in vectors and matrices start from 0 instead of 1 in this article. For a vector $\boldsymbol{a}$ of length k, the ith entry ($i \in \mathcal{Z}_k$) of $\boldsymbol{a}$ is denoted by $\boldsymbol{a}(i)$, and for a $k \times l$ matrix $\boldsymbol{A}$, the (i,j)th entry ($i \in \mathcal{Z}_k$ and $j \in \mathcal{Z}_l$) of $\boldsymbol{A}$ is denoted by $\boldsymbol{A}(i,j)$. A bijection $\boldsymbol{\pi} : \mathcal{Z}_k \to \mathcal{Z}_k$ is called a *permutation* on $\mathcal{Z}_k$, and is represented by a row vector $\boldsymbol{\pi} = (\boldsymbol{\pi}(0), \ldots, \boldsymbol{\pi}(k-1)) \in \mathcal{Z}_k^k$. Denote the *symmetric group* on $\mathcal{Z}_k$ by $\mathcal{S}_k = \left\{\boldsymbol{\pi} : \boldsymbol{\pi} \text{ is a permutation on } \mathcal{Z}_k\right\}$. The multiplication on the symmetric group, represented by "$\circ$", is the composition between mappings, that is, for any $\boldsymbol{\pi}_0, \boldsymbol{\pi}_1 \in \mathcal{S}_k$, $\boldsymbol{\pi}_0 \circ \boldsymbol{\pi}_1 = \Big(\boldsymbol{\pi}_0\big(\boldsymbol{\pi}_1(0)\big), \ldots, \boldsymbol{\pi}_0\big(\boldsymbol{\pi}_1(k-1)\big)\Big)$. The identity element of $\mathcal{S}_m$ is $\mathrm{id}_{\mathcal{Z}_k} = (0, \ldots, k-1)$. For any $\boldsymbol{\pi} \in \mathcal{S}_k$, the inverse of $\boldsymbol{\pi}$, denoted by $\mathrm{inv}(\boldsymbol{\pi})$, is the unique element in $\mathcal{S}_k$ such that $\mathrm{inv}(\boldsymbol{\pi}) \circ \boldsymbol{\pi} = \boldsymbol{\pi} \circ \mathrm{inv}(\boldsymbol{\pi}) = \mathrm{id}_{\mathcal{Z}_k}$. We use the notation "$\mathrm{inv}(\boldsymbol{\pi})$" instead of "$\boldsymbol{\pi}^{-1}$" in order to distinguish the inverse of a permutation from the inverse of a scalar or a matrix. For any proposition P, let $\mathbb{I}(\mathrm{P}) = 1$ if P is true and $\mathbb{I}(\mathrm{P}) = 0$ otherwise.

Denote the m components ($m \geqslant 2$) in an OofA experiment by $0, 1, \ldots, m-1$. Each run is represented by a $\boldsymbol{z} \in \mathcal{S}_m$, meaning that the component $\boldsymbol{z}(i)$ is arranged at the position i for every $i \in \mathcal{Z}_m$. On the other hand, its inverse permutation $\boldsymbol{x} = \mathrm{inv}(\boldsymbol{z})$ represents the *positions of components* (PofC), that is, $\boldsymbol{z}$ arranges the component i to the position $\boldsymbol{x}(i)$ for each $i \in \mathcal{Z}_m$. Thus, we call $\boldsymbol{x}$ the *PofC vector* corresponding to the run $\boldsymbol{z}$. For example, when $m = 3$, $\boldsymbol{z} = (2, 0, 1) \in \mathcal{S}_3$ is a possible run in an OofA experiment, with PofC vector $\mathrm{inv}(\boldsymbol{z}) = (1, 2, 0) \in \mathcal{S}_3$. Then, $\boldsymbol{z}$ arranges the components $0, 1, 2$ to the positions $1, 2, 0$, respectively. For any run $\boldsymbol{z} \in \mathcal{S}_m$ and any permutation $\boldsymbol{\pi} \in \mathcal{S}_m$, the product $\boldsymbol{\pi} \circ \boldsymbol{z}$ is the run obtained by relabeling the symbols in $\boldsymbol{z}$ according to $\boldsymbol{\pi}$, and the product $\boldsymbol{z} \circ \boldsymbol{\pi}$ is the run obtained by permuting the positions of the entries of $\boldsymbol{z}$ according to $\boldsymbol{\pi}$. For example, with $m = 3$, $\boldsymbol{z} = (2, 0, 1)$ and $\boldsymbol{\pi} = (0, 2, 1)$, $\boldsymbol{\pi} \circ \boldsymbol{z} = (1, 0, 2)$ can be obtained by interchanging the symbols "1" and "2" in $\boldsymbol{z}$, while $\boldsymbol{z} \circ \boldsymbol{\pi} = (2, 1, 0)$ can be obtained by interchanging the last two entries of $\boldsymbol{z}$.

Let $\mathcal{S}(N, m) = \left\{\left(\boldsymbol{z}_0^{\mathrm{T}}, \ldots, \boldsymbol{z}_{N-1}^{\mathrm{T}}\right)^{\mathrm{T}} : \boldsymbol{z}_0, \ldots, \boldsymbol{z}_{N-1} \in \mathcal{S}_m\right\}$, and call each $\boldsymbol{D} \in \mathcal{S}(N, m)$ an *OofA design* of N runs and m components. For example, the full OofA design $\boldsymbol{D}_m^{\mathrm{F}} \in \mathcal{S}(m!, m)$ contains each permutation in $\mathcal{S}_m$ exactly once as a row. For any OofA design $\boldsymbol{D} = \left(\boldsymbol{z}_0^{\mathrm{T}}, \ldots, \boldsymbol{z}_{N-1}^{\mathrm{T}}\right)^{\mathrm{T}} \in \mathcal{S}(N, m)$, define the PofC array of $\boldsymbol{D}$ as

$$\mathrm{inv}(\boldsymbol{D}) = \left(\mathrm{inv}(\boldsymbol{z}_0)^{\mathrm{T}}, \ldots, \mathrm{inv}(\boldsymbol{z}_{N-1})^{\mathrm{T}}\right)^{\mathrm{T}} \in \mathcal{S}(N, m),$$

and with any $\boldsymbol{\pi} \in \mathcal{S}_m$, denote

$$\boldsymbol{\pi} \circ \boldsymbol{D} = \begin{pmatrix} \boldsymbol{\pi} \circ \boldsymbol{z}_0 \\ \vdots \\ \boldsymbol{\pi} \circ \boldsymbol{z}_{N-1} \end{pmatrix} \in \mathcal{S}(N, m),$$
$$\boldsymbol{D} \circ \boldsymbol{\pi} = \begin{pmatrix} \boldsymbol{z}_0 \circ \boldsymbol{\pi} \\ \vdots \\ \boldsymbol{z}_{N-1} \circ \boldsymbol{\pi} \end{pmatrix} \in \mathcal{S}(N, m).$$

In fact, $\boldsymbol{\pi} \circ \boldsymbol{D}$ is the relabeling of $\boldsymbol{D}$ by $\boldsymbol{\pi}$, and $\boldsymbol{D} \circ \boldsymbol{\pi}$ is the column permutation of $\boldsymbol{D}$ by $\boldsymbol{\pi}$.

Under a linear regression model, the response at any run $\boldsymbol{z} \in \mathcal{S}_m$ is assumed to be $\mu(\boldsymbol{z}) + \varepsilon$, where ε is a random error,

$$\mu(\boldsymbol{z}) = \boldsymbol{f}(\boldsymbol{x})^{\mathrm{T}} \boldsymbol{\beta} \tag{1}$$

is the mean response at $\boldsymbol{z}$, $\boldsymbol{x} = \mathrm{inv}(\boldsymbol{z})$ is the PofC vector, $\boldsymbol{f} : \mathcal{S}_m \to \mathbb{R}^{p\times 1}$ is the regressor, and $\boldsymbol{\beta} \in \mathbb{R}^{p\times 1}$ is the unknown model parameter. Since the random errors at different runs are commonly assumed to be uncorrelated and homoscedastic, the regressor $\boldsymbol{f}$ basically specifies the linear model, and hence, we will use $\boldsymbol{f}$ to refer to this model. For an OofA design $\boldsymbol{D} \in \mathcal{S}(N, m)$ with PofC array $\boldsymbol{P} = \mathrm{inv}(\boldsymbol{D}) = \left(\boldsymbol{x}_0^{\mathrm{T}}, \ldots, \boldsymbol{x}_{N-1}^{\mathrm{T}}\right)^{\mathrm{T}}$, the model matrix of $\boldsymbol{D}$ under Model (1) is defined to be $\mathbf{F}_{\boldsymbol{f}}(\boldsymbol{D}) = \left(\boldsymbol{f}(\boldsymbol{x}_0), \ldots, \boldsymbol{f}(\boldsymbol{x}_{N-1})\right)^{\mathrm{T}} \in \mathbb{R}^{N\times p}$. For convenience, we call the rank of $\mathbf{F}_{\boldsymbol{f}}(\boldsymbol{D}_m^{\mathrm{F}})$ the rank of MOdel (1), and denote it by $\mathrm{rank}(\boldsymbol{f})$. Obviously, $\mathrm{rank}(\boldsymbol{f}) \leqslant p$, and when $\mathrm{rank}(\boldsymbol{f}) < p$, Model (1) is overparameterized. Two linear models $\boldsymbol{f}$ and $\boldsymbol{f}'$ are said to be *equivalent*, provided that the linear space spanned by the columns of $\mathbf{F}_{\boldsymbol{f}}(\boldsymbol{D}_m^{\mathrm{F}})$ is the same as that spanned by the columns of $\mathbf{F}_{\boldsymbol{f}'}(\boldsymbol{D}_m^{\mathrm{F}})$. In other words, $\boldsymbol{f}$ and $\boldsymbol{f}'$ are equivalent if and only if they can express each other through linear transformations. By the theory of linear regression, equivalent models are the same in fitting and predicting. Indeed, the interpretations and selections of respective model parameters of equivalent models, which depend on the concrete parameterization, can be quite different. However, in many real case studies involving OofA effects (Mee 2020; Yang, Sun, and Xu 2021; Xiao et al. 2024), the main focus is on finding the optimal order that produces a desirable response value, in which case the most concerned perspective is the precision of prediction.

As Stokes and Xu (2022) pointed out, Model (1) is a very flexible form including many classical models as special cases, for example, the PWO model (Van Nostrand 1995) and the CP model (Yang, Sun, and Xu 2021). However, Model (1) is too general, so few theoretical results can be obtained based on it. Most of the popularly-used models are equivalent to models possessing some kind of symmetry. For example, in the overparameterized version of the CP model (Yang, Sun, and Xu 2021, Model (1)), the mean response has the form

$$\beta_0 + \sum_{j\in\mathcal{Z}_m}\sum_{i\in\mathcal{Z}_m}\mathbb{I}(\boldsymbol{x}(j)=i)\cdot\beta_{j,i} \tag{2}$$

for any run with PofC vector $\boldsymbol{x} \in \mathcal{S}_m$. Intuitively, this model seems symmetric, since the regressor can be written into the form $\boldsymbol{f}(\boldsymbol{x}) = \left(1, \boldsymbol{f}_1(\boldsymbol{x}(0))^{\mathrm{T}}, \ldots, \boldsymbol{f}_1(\boldsymbol{x}(m-1))^{\mathrm{T}}\right)^{\mathrm{T}}$, where the concrete expression of $\boldsymbol{f}_1$ will be given later in Example 2. That is, all the components play the same role in Model (2). In contrast, in the CP model with the baseline constraint, the mean response has the form

$$\beta_0 + \sum_{j\in\mathcal{Z}_m\backslash\{j_0\}}\sum_{i\in\mathcal{Z}_m\backslash\{i_0\}}\mathbb{I}(\boldsymbol{x}(j)=i)\cdot\beta_{j,i} \tag{3}$$

for any PofC vector $\boldsymbol{x} \in \mathcal{S}_m$, where the baseline component $j_0 \in \mathcal{Z}_m$ and the baseline position $i_0 \in \mathcal{Z}_m$ are preselected arbitrarily. Such a model seems not symmetric, because the role of the baseline component j_0 is different from the roles of the other components. However, this model is symmetric essentially in the sense that it is equivalent to Model (2). In situations when all the m components and all the m positions are of the same importance, there is no specific reason to select any $j_0 \in \mathcal{Z}_m$ to be the baseline component or to select any $i_0 \in \mathcal{Z}_m$ to be the baseline position, so the overparameterized but symmetric model form (2) seems more plausible. As a counterexample, if a model has the mean response of the form $\beta_\emptyset + \beta_0\boldsymbol{x}(0) + \beta_1\boldsymbol{x}(1)^2 + \beta_2\sin(\boldsymbol{x}(2)) + \beta_3\exp(\boldsymbol{x}(3)) + \cdots$ for any PofC vector $\boldsymbol{x} \in \mathcal{S}_m$, then this model is not symmetric at all, because the components appear in different forms in the model, that is, the roles of these components are different. Such a model is hard to study and less useful in practice. Therefore, we will focus on a broad subclass of linear models which includes the classical models as special cases in the sense of equivalence and meanwhile possesses some kind of symmetry. For any $m \in \mathbb{N}_+$ and $t \in \{0, 1, \ldots, m\}$, let $\mathcal{P}_m^t = \{(\boldsymbol{\pi}(0), \ldots, \boldsymbol{\pi}(t-1)) : \boldsymbol{\pi} \in \mathcal{S}_m\} = \{(a_0, \ldots, a_{t-1}) : a_0, \ldots, a_{t-1} \in \mathcal{Z}_m \text{ are distinct}\}$, whose cardinality is $P_m^t = \mathrm{Card}(\mathcal{P}_m^t) = m!/(m-t)! = \prod_{i\in\mathcal{Z}_t}(m-i)$.

Definition 1. Model (1) is called a τ-way symmetric linear model, if there exists a $\tau \in \{0, \ldots, m\}$ such that for any run $\boldsymbol{z} \in \mathcal{S}_m$ with $\mathrm{inv}(\boldsymbol{z}) = \boldsymbol{x} = (\boldsymbol{x}(0), \ldots, \boldsymbol{x}(m-1))$,

$$\begin{aligned}\mu(\boldsymbol{z}) &= \boldsymbol{f}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\beta}\\ &= \sum_{k=0}^{\tau}\sum_{0\leqslant j_0<\cdots<j_{k-1}<m}\boldsymbol{f}_k(\boldsymbol{x}(j_0), \ldots, \boldsymbol{x}(j_{k-1}))^{\mathrm{T}}\boldsymbol{\beta}_{(j_0,\ldots,j_{k-1})},\end{aligned} \tag{4}$$

where

(i) $\boldsymbol{f}_0$ is a constant nonzero number (usually $\boldsymbol{f}_0 = 1$), $p_0 = 1$ and $\boldsymbol{\beta}_\emptyset \in \mathbb{R}$ is an unknown parameter, if the model contains the intercept term; otherwise, $\boldsymbol{f}_0$ and $\boldsymbol{\beta}_\emptyset$ are ignored and $p_0 = 0$;
(ii) for each $k \in \{1, \ldots, \tau\}$, $\boldsymbol{f}_k : \mathcal{P}_m^k \to \mathbb{R}^{p_k\times 1}$, $p_k \in \mathbb{N}$, and for any $\boldsymbol{\pi} \in \mathcal{S}_k$, there exists a permutation matrix $\boldsymbol{S} \in \{0,1\}^{p_k\times p_k}$ such that, for any $(a_0, \ldots, a_{k-1}) \in \mathcal{P}_m^k$, $\boldsymbol{f}_k(a_{\boldsymbol{\pi}(0)}, \ldots, a_{\boldsymbol{\pi}(k-1)}) = \boldsymbol{S}\cdot\boldsymbol{f}_k(a_0, \ldots, a_{k-1})$;
(iii) for each $k \in \{1, \ldots, \tau\}$ and $0 \leqslant j_0 < \cdots < j_{k-1} < m$, $\boldsymbol{\beta}_{(j_0,\ldots,j_{k-1})} \in \mathbb{R}^{p_k\times 1}$ is a vector of unknown parameters;
(iv) $p_\tau > 0$, and the length of $\boldsymbol{\beta}$ is $p = \sum_{k=0}^{\tau}\binom{m}{k}p_k$.

For brevity, we also call Model (4) a "symmetric model". Roughly speaking, the form of Model (4) is already symmetric, since all the components play the same role in it. However, consider $k \in \{2, \ldots, \tau\}$ and integers $0 \leqslant j_0 < \cdots < j_{k-1} < m$. For any PofC vector $\boldsymbol{x} \in \mathcal{S}_m$, $\boldsymbol{f}_k\big(\boldsymbol{x}(j_0), \ldots, \boldsymbol{x}(j_{k-1})\big)$ is a column subvector of $\boldsymbol{f}(\boldsymbol{x})$. For a permutation $\boldsymbol{\pi} \in \mathcal{S}_m$, $\boldsymbol{f}_k\big(\boldsymbol{x}(j_0), \ldots, \boldsymbol{x}(j_{k-1})\big) = \boldsymbol{f}_k\Big((\boldsymbol{x}\circ\boldsymbol{\pi})\big(\mathrm{inv}(\boldsymbol{\pi})(j_0)\big), \ldots, (\boldsymbol{x}\circ\boldsymbol{\pi})\big(\mathrm{inv}(\boldsymbol{\pi})(j_{k-1})\big)\Big)$, but we don't have $\mathrm{inv}(\boldsymbol{\pi})(j_0) < \cdots < \mathrm{inv}(\boldsymbol{\pi})(j_{k-1})$, so we need a permutation matrix independent of $\boldsymbol{x}$ which transforms $\boldsymbol{f}_k\big(\boldsymbol{x}(j_0), \ldots, \boldsymbol{x}(j_{k-1})\big)$ into a column subvector of $\boldsymbol{f}(\boldsymbol{x}\circ\boldsymbol{\pi})$. Therefore, Condition (ii) is required in Definition 1, which guarantees that for any $\boldsymbol{\pi} \in \mathcal{S}_m$, there exists some permutation matrix $\boldsymbol{S}_{\boldsymbol{\pi}} \in \{0,1\}^{p\times p}$ such that $\boldsymbol{f}(\boldsymbol{x}\circ\boldsymbol{\pi}) = \boldsymbol{S}_{\boldsymbol{\pi}}\boldsymbol{f}(\boldsymbol{x})$ for any $\boldsymbol{x} \in \mathcal{S}_m$. This permutation-covariant property is precisely what we refer to by "symmetric". Specially, when $\tau = 0$, Model (4) only contains the intercept standing for the overall mean, and when $\tau \leqslant 1$, Model (4) naturally satisfies Condition (ii). The following examples illustrate how to re-express the (tapered-effect) PWO model and the CP model in their equivalent symmetric forms. Several more examples corresponding to other existing linear models for OofA experiments are provided in Supplementary Material S1, along with some new models. For convenience, we summarize these symmetric models in Table 1. Except the NN model, all the other symmetric models are overparameterized, since in order to achieve the symmetry, some extra model terms are needed, leading to $\mathrm{rank}(\boldsymbol{f}) < p$ in Model (4). For a more comprehensive review about models for OofA experiments, please refer to Mee (2024) and Piepho and Williams (2021). Also refer to Xiao and Xu (2021), Xiao et al. (2024), Huang and Phoa (2024) for more modeling techniques, where linear models depending on the designs and Gaussian process models are adopted.

Table 1. A summary of τ-way symmetric linear models with m components.

Model	τ	p	Example	Reference
sPWO	2	$1+m(m-1)$	1	Van Nostrand (1995)
sTPWO	2	$1+m(m-1)$	1	Peng, Mukerjee, and Lin (2019)
NN	2	$m(m-1)$	S4	* Piepho and Williams (2021)
Symmetrized PWOD	2	$1+m(m-1)$	S1	Chen et al. (2023)
Symmetrized TriPWO	3	$1+P_m^2+P_m^3$	S2	Mee (2020)
Symmetrized 2FI PWO	4	$1+P_m^2+P_m^3+6\binom{m}{4}$	S2	Mee (2024)
τ-way OofA	τ	$1+P_m^\tau$	S3	* Lin and Peng (2019)
CP	1	$1+m^2$	2	* Yang, Sun, and Xu (2021)
CPP	1	$1+m(m-1)$	S5	* This article
sFP	1	$1+m$	S6	Stokes and Xu (2022)
sQP	1	$1+2m$	S6	Stokes and Xu (2022)
sSP	2	$1+2m+\binom{m}{2}$	S7	Stokes and Xu (2022)
sSC	3	$m+\binom{m}{2}+\binom{m}{3}$	S8	Piepho and Williams (2021)
sFC	3	$m+3\binom{m}{2}+\binom{m}{3}$	S8	Piepho and Williams (2021)
CP(τ)	τ	$\binom{m}{\tau}P_m^\tau$	S10	* This article

NOTE: The "*" before the reference indicates that the original model in the reference is already symmetric.

Example 1. The PWO model proposed by Van Nostrand (1995) is based on the relative positions between components. Precisely, for any run $\boldsymbol{z} \in \mathcal{S}_m$ with PofC vector $\boldsymbol{x} = \mathrm{inv}(\boldsymbol{z})$, the PWO factor corresponding to a pair of distinct components $0 \leqslant j_0 < j_1 \leqslant m-1$, denoted by $\delta_{\mathrm{PWO}}(\boldsymbol{x}(j_0), \boldsymbol{x}(j_1))$, is defined to be 1 if $\boldsymbol{x}(j_0) < \boldsymbol{x}(j_1)$, and to be -1 if $\boldsymbol{x}(j_0) > \boldsymbol{x}(j_1)$. Then, the corresponding mean response under the PWO model has the form

$$\beta_0 + \sum_{0\leqslant j_0<j_1\leqslant m-1} \delta_{\mathrm{PWO}}(\boldsymbol{x}(j_0), \boldsymbol{x}(j_1)) \cdot \beta_{(j_0,j_1)}.$$

The regressor of the PWO model is

$$\boldsymbol{f}_{\mathrm{PWO}}(\boldsymbol{x}) = \Big(1, \delta_{\mathrm{PWO}}\big(\boldsymbol{x}(0), \boldsymbol{x}(1)\big), \ldots, \delta_{\mathrm{PWO}}\big(\boldsymbol{x}(m-2), \boldsymbol{x}(m-1)\big)\Big)^{\mathrm{T}}$$

for any $\boldsymbol{x} \in \mathcal{S}_m$. Peng, Mukerjee, and Lin (2019) generalized the PWO model to accommodate possible tapered-effects, in which the regressor is

$$\boldsymbol{f}_{\mathrm{TPWO}}(\boldsymbol{x}) = \Big(1, \delta_{\mathrm{TPWO}}\big(\boldsymbol{x}(0), \boldsymbol{x}(1)\big), \ldots, \delta_{\mathrm{TPWO}}\big(\boldsymbol{x}(m-2), \boldsymbol{x}(m-1)\big)\Big)^{\mathrm{T}} \tag{5}$$

for any $\boldsymbol{x} \in \mathcal{S}_m$, where $\delta_{\mathrm{TPWO}}(a_0, a_1) = c_{|a_1-a_0|}$ if $a_0 < a_1$, and $\delta_{\mathrm{TPWO}}(a_0, a_1) = -c_{|a_1-a_0|}$ if $a_0 > a_1$, and $c_1 \geqslant \cdots \geqslant c_{m-1} \geqslant 0$ are $(m-1)$ pre-defined parameters. We refer to Model (5) as the tapered-effect PWO (TPWO) model. Specifically, when $c_1 = \cdots = c_{m-1} = 1$, the TPWO model degenerates to the PWO model. When $c_1 > 0$, $\boldsymbol{f}_{\mathrm{TPWO}}(\mathrm{id}_{\mathcal{Z}_m})$ consists of nonnegative entries, but $\boldsymbol{f}_{\mathrm{TPWO}}((m-1, m-2, \ldots, 0))$ contains $-c_1$, so Condition (ii) of Definition 1 is violated, and Model (5) is not symmetric. Next, we re-express the TPWO model in its equivalent symmetric form. In Model (4), take $\tau = 2$, $p_0 = 1$, $p_1 = 0$, $p_2 = 2$ and $p = 1 + m(m-1)$, and take $\boldsymbol{f}_2$ as

$$\boldsymbol{f}_2(a_0, a_1) = (\delta_{\mathrm{TPWO}}(a_0, a_1), -\delta_{\mathrm{TPWO}}(a_0, a_1))^{\mathrm{T}} \tag{6}$$

for any $(a_0, a_1) \in \mathcal{P}_m^2$. Obviously, the above model satisfies Condition (ii) of Definition 1, since in Condition (ii), when $k = \tau = 2$ and $\boldsymbol{\pi} = (1, 0) \in \mathcal{S}_2$, the corresponding permutation matrix $\boldsymbol{S} \in \{0, 1\}^{2\times 2}$ exists, with $\boldsymbol{S}(0, 0) = \boldsymbol{S}(1, 1) = 0$ and $\boldsymbol{S}(0, 1) = \boldsymbol{S}(1, 0) = 1$. Therefore, we obtain a 2-way symmetric model $\boldsymbol{f}_{\mathrm{sTPWO}}$, called the sTPWO model. Let

$$\boldsymbol{C} = \begin{pmatrix} 1 & \boldsymbol{0}_{1\times m(m-1)} \\ \boldsymbol{0}_{\binom{m}{2}\times 1} & \mathbf{I}_{\binom{m}{2}} \otimes (1, -1) \end{pmatrix}, \tag{7}$$

where "$\otimes$" represents the Kronecker product. Then, $\boldsymbol{f}_{\mathrm{sTPWO}} = \boldsymbol{C}^{\mathrm{T}}\boldsymbol{f}_{\mathrm{TPWO}}$, so the sTPWO model is equivalent to the TPWO model. Let $\boldsymbol{\beta}_{\mathrm{TPWO}}$ and $\boldsymbol{\beta}_{\mathrm{sTPWO}}$ be the respective parameter vectors under the TPWO model and the sTPWO model, then $\boldsymbol{\beta}_{\mathrm{TPWO}} = \boldsymbol{C}\boldsymbol{\beta}_{\mathrm{sTPWO}}$. Specifically, when $c_1 = \cdots = c_{m-1} = 1$, the sTPWO model is called the sPWO model, which is equivalent to the PWO model.

Example 2. The CP model (2) proposed by Yang, Sun, and Xu (2021) is based on the absolute positions of components, and it is a 1-way symmetric model satisfying Definition 1. It can be obtained from Model (4) by taking $\tau = 1$, $p_0 = 1$, $p_1 = m$ and $p = 1 + m^2$, and taking $\boldsymbol{f}_1$ as $\boldsymbol{f}_1(a) = (\mathbb{I}(a = 0), \ldots, \mathbb{I}(a = m-1))^{\mathrm{T}}$ for any $a \in \mathcal{Z}_m$. This model is of rank $1 + (m-1)^2$. Please refer to Example S9 in Supplementary Material S1 for the verification of the equivalence between the CP models (3) and (2) with and without the baseline constraint.

3. Universally Optimal Designs

Under given models, an important class of criteria for assessing experimental designs is the various information-based optimality criteria, including the D- and A-optimality criteria. In this Section, we mainly discuss the optimality of COAs under symmetric linear models. As a class of OofA designs, COAs were first proposed by Yang, Sun, and Xu (2021) and then generalized by Zhao, Li, and Zhao (2021).

Definition 2 (Zhao, Li, and Zhao 2021). For $m, \lambda \in \mathbb{N}_+$, $t \in \{0, \ldots, m\}$ and $N = \lambda P_m^t$, a matrix $\boldsymbol{D} \in \mathcal{S}(N, m)$ is called a component orthogonal array (COA) of N runs, m components, strength t and index λ, denoted as a COA(N, m, t), if in any distinct t columns of $\boldsymbol{D}$, each element of $\mathcal{P}_m^t$ appears for exactly λ times as a row vector.

It is easy to know that, if $\boldsymbol{D}$ is a COA(N, m, t), then $\boldsymbol{D}$ is also a COA(N, m, t') for any $t' \in \{0, \ldots, t\}$. Therefore, any property that is possessed by every COA of strength t is also possessed by every COA of any higher strength. Specifically, any $\boldsymbol{D} \in \mathcal{S}(N, m)$ is a COA$(N, m, 0)$. When the strength $t = 1$, the only requirement for an OofA design to be a COA$(N, m, 1)$ is that, in each column, all m components appear equally often. When the strength $t = 2$, a COA$(N, m, 2)$ is exactly the COA defined by Yang, Sun, and Xu (2021). Moreover, a COA$(N, m, m-1)$ must be a COA(N, m, m), which consists of $N/m!$ replications of the full OofA design $\boldsymbol{D}_m^{\mathrm{F}}$. Besides, COAs possess the following property.

Proposition 1. For any OofA design $\boldsymbol{D} \in \mathcal{S}(N, m)$ and any $\boldsymbol{\pi} \in \mathcal{S}_m$, if one of $\boldsymbol{D}$, $\mathrm{inv}(\boldsymbol{D})$, $\boldsymbol{\pi} \circ \boldsymbol{D}$ and $\boldsymbol{D} \circ \boldsymbol{\pi}$ is a COA(N, m, t), so are the other three designs.

Proposition 1 indicates that requiring an OofA design to be a COA is equivalent to requiring its PofC array to be a COA, and whether or not an OofA design is a COA is not affected by any relabeling or column permutation.

In order to develop the optimality theory for COAs, we introduce some concepts. Denote the set of all probability measures on $\mathcal{S}_m$ by $\mathcal{S}(\infty, m)$. We call each $\xi \in \mathcal{S}(\infty, m)$ an *OofA design measure*, which is also known as an approximate design in the literature on optimal designs. For any OofA design $\boldsymbol{D} \in \mathcal{S}(N, m)$, the design measure of $\boldsymbol{D}$, denoted by $\xi_{\boldsymbol{D}}$, has mass $\xi_{\boldsymbol{D}}(\boldsymbol{z}) = k_{\boldsymbol{z}}/N$ on any $\boldsymbol{z} \in \mathcal{S}_m$, where $k_{\boldsymbol{z}}$ is the number of times for which $\boldsymbol{z}$ appears in $\boldsymbol{D}$. Under Model (1), the *per-run information matrix* corresponding to an OofA design measure ξ is

$$\mathbf{M}_{\boldsymbol{f}}(\xi) = \sum_{z \in \mathcal{S}_m} \xi(\boldsymbol{z}) \cdot \boldsymbol{f}(\mathrm{inv}(\boldsymbol{z}))\boldsymbol{f}(\mathrm{inv}(\boldsymbol{z}))^{\mathrm{T}} \in \mathbb{R}^{p \times p}.$$

The design measure ξ is said to be *nonsingular* if $\mathrm{rank}\left(\mathbf{M}_{\boldsymbol{f}}(\xi)\right) = \mathrm{rank}(\boldsymbol{f})$, and *singular* if $\mathrm{rank}\left(\mathbf{M}_{\boldsymbol{f}}(\xi)\right) < \mathrm{rank}(\boldsymbol{f})$. The set of all information matrices

$$\mathcal{M}_{\boldsymbol{f}} = \left\{\mathbf{M}_{\boldsymbol{f}}(\xi) : \xi \in \mathcal{S}(\infty, m)\right\} \subseteq \mathbb{R}^{p \times p}$$

is a convex set. For an OofA design $\boldsymbol{D}$, we write $\mathbf{M}_{\boldsymbol{f}}(\boldsymbol{D}) = \mathbf{M}_{\boldsymbol{f}}(\xi_{\boldsymbol{D}})$ for brevity.

Let $\Phi : \mathcal{M}_{\boldsymbol{f}} \to [-\infty, +\infty]$ be an optimality criterion to be maximized. An OofA design measure $\xi \in \mathcal{S}(\infty, m)$ is Φ-*optimal*, provided that $\mathbf{M}_{\boldsymbol{f}}(\xi)$ maximizes Φ over $\mathcal{M}_{\boldsymbol{f}}$. An OofA design $\boldsymbol{D} \in \mathcal{S}(N, m)$ is Φ-*optimal*, provided that $\Phi\left(\mathbf{M}_{\boldsymbol{f}}(\boldsymbol{D})\right)$ is maximized by $\boldsymbol{D}$ over $\mathcal{S}(N, m)$. Moreover, $\boldsymbol{D}$ is said to *have a* Φ-*optimal design measure*, provided that $\xi_{\boldsymbol{D}}$ is Φ-optimal. Therefore, for $\boldsymbol{D}$, to have a Φ-optimal design measure is stronger than to be Φ-optimal. For example, under the setting of Theorem 3 to be presented later, when a $\mathrm{COA}(N, m, t)$ does not exist, no OofA design with N runs has a D-optimal design measure, although there must exist a D-optimal OofA design with N runs due to the finiteness of $\mathcal{S}(N, m)$.

Below we introduce the permutation-invariant optimality criteria and the universal optimality (Kiefer 1975); please refer to Pukelsheim (2006) for further explanations and discussions.

Definition 3. Under Model (1), a function $\Phi : \mathcal{M}_{\boldsymbol{f}} \to [-\infty, +\infty]$ is called a permutation-invariant optimality criterion, provided

(i) Φ is nondecreasing: for any $\boldsymbol{M}_0, \boldsymbol{M}_1 \in \mathcal{M}_{\boldsymbol{f}}$ such that $\boldsymbol{M}_1 - \boldsymbol{M}_0$ is nonnegative definite, $\Phi(\boldsymbol{M}_1) \geqslant \Phi(\boldsymbol{M}_0)$;
(ii) Φ is concave: for any $\boldsymbol{M}_0, \boldsymbol{M}_1 \in \mathcal{M}_{\boldsymbol{f}}$ and $a \in (0, 1)$, $\Phi(a\boldsymbol{M}_0 + (1-a)\boldsymbol{M}_1) \geqslant a\Phi(\boldsymbol{M}_0) + (1-a)\Phi(\boldsymbol{M}_1)$;
(iii) Φ is invariant to permutation: for any $\boldsymbol{M} \in \mathcal{M}_{\boldsymbol{f}}$ and any permutation matrix $\boldsymbol{S} \in \{0, 1\}^{p \times p}$ such that $\boldsymbol{S}\boldsymbol{M}\boldsymbol{S}^{\mathrm{T}} \in \mathcal{M}_{\boldsymbol{f}}$, $\Phi(\boldsymbol{M}) = \Phi(\boldsymbol{S}\boldsymbol{M}\boldsymbol{S}^{\mathrm{T}})$.

In Definition 3, Condition (i) is quite natural since our purpose is to find design measures having "large" information matrices. Condition (ii) reflects that all entries of the parameter vector are of the same importance, so the criterion value should remain unchanged if only the entries of the parameter vector are permuted but the design measure is not changed. Condition (ii) is required for technical convenience. Practically, many commonly-used criteria, including the T-, D-, A-, and E-criteria, are permutation-invariant optimality criteria satisfying Definition 3 (Pukelsheim 2006, chap.'s 6 & 13).

An OofA design measure $\xi \in \mathcal{S}(\infty, m)$ (or an OofA design $\boldsymbol{D} \in \mathcal{S}(N, m)$) is *universally optimal*, provided that ξ (or $\boldsymbol{D}$) is Φ-optimal for every permutation-invariant optimality criterion Φ. Moreover, an OofA design $\boldsymbol{D} \in \mathcal{S}(N, m)$ is said to *have a universally optimal design measure* provided that $\xi_{\boldsymbol{D}}$ is universally optimal.

Inspired by Theorem 1 in Peng, Mukerjee, and Lin (2019), whose proof is similar to the routine in universal optimality theory (Kiefer 1975), we obtain the following result.

Theorem 1. Under the τ-way symmetric linear model (4), any $\mathrm{COA}(N, m, t)$ with $t = \min\{2\tau, m\}$ has a universally optimal design measure.

We have seen from Section 2 that all popularly-used linear models for OofA experiments are equivalent to symmetric models, and then Theorem 1 guarantees that for any $t \in \{0, \dots, m\}$, COAs of strength t have optimal design measures with respect to various optimality criteria under all τ-way symmetric models for any $\tau \in \{0, \dots, \lfloor t/2 \rfloor\}$, where $\lfloor a \rfloor$ represents the largest integer not exceeding a for any $a \in \mathbb{R}$. Specially, the full OofA design has a universally optimal design measure under any symmetric linear model. Note that, for an odd $t \leqslant m-2$, Theorem 1 cannot distinguish the performance of a COA of strength t from that of a COA of strength $t-1$. That is, for $\tau \in \{0, \dots, (t-1)/2\}$, both a $\mathrm{COA}(N, m, t)$ and a $\mathrm{COA}(N', m, t-1)$ are universally optimal under all τ-way symmetric models, but for $\tau \in \{(t-1)/2+1, \dots, m\}$, their performances under τ-way symmetric models are not guaranteed by Theorem 1. Nevertheless, the numerical results in Supplementary Material S5 indicate that the efficiency of COAs of strength 3 may be between COAs of strengths 2 and 4. In practice, higher-order interaction effects are seldom considered, then usually 1-way or 2-way symmetric models are used, including the 1-way CP, sFP, and sQP models and the 2-way sTPWO and sSP models in Table 1. Therefore, to guarantee the optimality of a COA, the required strength is usually 2 or 4, which is not too high.

However, since symmetric models are often overparameterized, some modifications have to be made to the commonly-used criteria. Here, we only focus on an important class of criteria called the matrix mean criteria (Pukelsheim 2006, chap. 6), which includes the well-known T-, D-, A-, and E-criteria. Under Model (1), suppose $\boldsymbol{\beta} \in \mathbb{R}^{p \times 1}$ and $\mathrm{rank}(\boldsymbol{f}) = r$, where $r \leqslant p$. Take an arbitrary per-run information matrix $\boldsymbol{M} \in \mathcal{M}_{\boldsymbol{f}}$, and let $\boldsymbol{\eta}(\boldsymbol{M}) = (\eta_0(\boldsymbol{M}), \dots, \eta_{p-1}(\boldsymbol{M})) \in \mathbb{R}^p$ be the vector of descending eigenvalues of $\boldsymbol{M}$. Then, we have $\eta_0(\boldsymbol{M}) \geqslant \cdots \geqslant \eta_{r-1}(\boldsymbol{M}) \geqslant \eta_r(\boldsymbol{M}) = \cdots = \eta_{p-1}(\boldsymbol{M}) = 0$. Similar to Kong, Yuan, and Zheng (2021, sec. 7), for any $u \in [-\infty, 1]$, we can define the reduced-rank version of the u-matrix mean criterion with respect to $\boldsymbol{M}$ to be

$$\Phi_u(\boldsymbol{M}) = \begin{cases} \eta_{r-1}(\boldsymbol{M}), & \text{if } u = -\infty, \\ \left(\prod_{i \in \mathcal{Z}_r} \eta_i(\boldsymbol{M})\right)^{1/r}, & \text{if } u = 0, \\ \left(\frac{1}{r}\sum_{i \in \mathcal{Z}_r} \eta_i(\boldsymbol{M})^u\right)^{1/u}, & \text{if } u \in (-\infty, 1] \setminus \{0\}, \end{cases}$$

where we consider $0^{-1} = \infty$ and $\infty^{-1} = 0$. Specifically, by taking u to be $1, 0, -1$, and $-\infty$, respectively, we obtain the reduced-rank versions of the T-, D-, A- and E-optimality criteria. The above matrix mean criteria all satisfy Definition 3; precisely, we have the following property.

Proposition 2. For any $u \in [-\infty, 1]$, the u-matrix mean criterion Φ_u on $\mathcal{M}_{\boldsymbol{f}}$ is a permutation-invariant optimality criterion satisfying Definition 3. Furthermore, when $u \in (-\infty, 1)$, the criterion Φ_u is strictly concave on

$$\mathcal{M}_{\boldsymbol{f}}^{+} = \left\{\boldsymbol{M} : \boldsymbol{M} \in \mathcal{M}_{\boldsymbol{f}} \text{ and } \operatorname{rank}(\boldsymbol{M}) = \operatorname{rank}(\boldsymbol{f})\right\}.$$

Remark 1. In Proposition 2, the "strict concavity" of Φ_u means that, for any real number $a \in (0, 1)$, and any $\boldsymbol{M}_0, \boldsymbol{M}_1 \in \mathcal{M}_{\boldsymbol{f}}^{+}$ such that $\boldsymbol{M}_0 \neq b\boldsymbol{M}_1$ for any $b > 0$, we have $\Phi_u(a\boldsymbol{M}_0 + (1 - a)\boldsymbol{M}_1) > a\Phi_u(\boldsymbol{M}_0) + (1 - a)\Phi_u(\boldsymbol{M}_1)$. Moreover, Proposition 2 is true for any linear model $\boldsymbol{f}$ of the form (1), not only for OofA experiments.

Guaranteed by Theorem 1 and Proposition 2, under a symmetric model, the design measure of a COA of enough strength is Φ_u-optimal simultaneously for any $u \in [-\infty, 1]$, and specifically, is T-, D-, A-, and E-optimal, simultaneously. Another important conclusion from Proposition 2 is that, for $u \in (-\infty, 1)$, $\mathbf{M}_{\boldsymbol{f}}(\boldsymbol{D}_m^{\mathrm{F}})$ is the unique maximizer of Φ_u on $\mathcal{M}_{\boldsymbol{f}}$, guaranteed by the strict concavity of Φ_u on $\mathcal{M}_{\boldsymbol{f}}^{+}$ and the fact that $\boldsymbol{D}_m^{\mathrm{F}}$ is a COA$(m!, m, m)$. Note that, though the optimal per-run information matrix is unique, there can exist multiple different Φ_u-optimal design measures.

Since symmetric models are often overparameterized, the above reduced-rank versions of the matrix mean criteria are often difficult to interpret. Therefore, we introduce some more practical criteria to assess OofA designs from the perspectives of prediction and estimation, respectively.

From the perspective of prediction, we desire a design that minimizes the average prediction variance. Formally, under Model (1), we want to find an OofA design measure ξ that maximizes

$$\Phi_{\mathrm{I}}(\mathbf{M}_{\boldsymbol{f}}(\xi)) = \begin{cases} -\frac{1}{m!}\sum_{\boldsymbol{x} \in \mathcal{S}_m} \boldsymbol{f}(\boldsymbol{x})^{\mathrm{T}} \left(\mathbf{M}_{\boldsymbol{f}}(\xi)\right)^{-} \boldsymbol{f}(\boldsymbol{x}), \\ \qquad \text{if } \operatorname{rank}(\mathbf{M}_{\boldsymbol{f}}(\xi)) = \operatorname{rank}(\boldsymbol{f}), \\ -\infty, \\ \qquad \text{if } \operatorname{rank}(\mathbf{M}_{\boldsymbol{f}}(\xi)) < \operatorname{rank}(\boldsymbol{f}), \end{cases}$$

where $\left(\mathbf{M}_{\boldsymbol{f}}(\xi)\right)^{-}$ is a generalized inverse of $\mathbf{M}_{\boldsymbol{f}}(\xi)$. This is exactly the well-known I-optimality criterion, which is not permutation-invariant in general.

Theorem 2. Under the τ-way symmetric linear model (4), any COA(N, m, t) with $t = \min\{2\tau, m\}$ has an I-optimal design measure.

A natural corollary of Theorem 2 is that the full OofA design has an I-optimal design measure under any symmetric model. If a linear model $\boldsymbol{f}$ is equivalent to a symmetric model $\boldsymbol{f}'$, then $\boldsymbol{f}$ and $\boldsymbol{f}'$ perform exactly the same on prediction, so by Theorem 2, a COA of enough strength minimizes the average prediction variance under model $\boldsymbol{f}$, no matter whether $\boldsymbol{f}$ is overparameterized or not. For example, a COA of strength 4 is I-optimal under both the sTPWO and the TPWO model in Example 1, as well as the NN model in Example S4.

From the perspective of parameter estimation, we need another more direct way to define optimality criteria for overparameterized models. For Model (1) with $r = \operatorname{rank}(\boldsymbol{f}) \leqslant p$, a usual interest is in the estimation of the linear combination $\boldsymbol{C\beta}$ of the parameter, where $\boldsymbol{C} \in \mathbb{R}^{r \times p}$ has row rank r, and $\boldsymbol{C\beta}$ is estimable under the full design $\boldsymbol{D}_m^{\mathrm{F}}$. For instance, under the sTPWO model in Example 1, an appealing such matrix $\boldsymbol{C}$ is the one in (7), since in this case, $\boldsymbol{C\beta}$ is exactly the parameter vector under the TPWO model. For any nonsingular OofA design measure ξ, by the theory of linear models, the variance of the least-square estimator of $\boldsymbol{C\beta}$ is proportional to $\boldsymbol{C}\left(\mathbf{M}_{\boldsymbol{f}}(\xi)\right)^{-}\boldsymbol{C}^{\mathrm{T}}$, which is invertible and is free of the choice of the generalized inverse $\left(\mathbf{M}_{\boldsymbol{f}}(\xi)\right)^{-}$. Therefore, we can take

$$\mathbf{M}_{\boldsymbol{f},\boldsymbol{C}}(\xi) = \left(\boldsymbol{C}\mathbf{M}_{\boldsymbol{f}}(\xi)^{-}\boldsymbol{C}^{\mathrm{T}}\right)^{-1}$$

to be the per-run information matrix of the design measure ξ with respect to $\boldsymbol{C\beta}$. Let $\mathcal{M}_{\boldsymbol{f},\boldsymbol{C}} = \left\{\left(\boldsymbol{C}\boldsymbol{M}^{-}\boldsymbol{C}^{\mathrm{T}}\right)^{-1} : \boldsymbol{M} \in \mathcal{M}_{\boldsymbol{f}}^{+}\right\}$, which is a convex subset of $\mathbb{R}^{r \times r}$. Then, the performance of any nonsingular OofA design measure ξ can be quantified by the u-matrix mean optimality criterion $\Phi_u(\mathbf{M}_{\boldsymbol{f},\boldsymbol{C}}(\xi))$, where $u \in [-\infty, 1]$. For convenience, a nonsingular OofA design measure ξ is said to be Φ_u*-optimal about* $\boldsymbol{C}$, provided $\mathbf{M}_{\boldsymbol{f},\boldsymbol{C}}(\xi)$ maximizes Φ_u over $\mathcal{M}_{\boldsymbol{f},\boldsymbol{C}}$. Specifically, by taking u to be $1, 0, -1$, and $-\infty$, respectively, we obtain the T-, D-, A- and E-optimality criteria about $\boldsymbol{C}$, as follows:

$$\begin{aligned} \Phi_{\mathrm{T}}(\boldsymbol{M}) &= \frac{\operatorname{tr}(\boldsymbol{M})}{r}, \\ \Phi_{\mathrm{D}}(\boldsymbol{M}) &= (\det(\boldsymbol{M}))^{1/r}, \\ \Phi_{\mathrm{A}}(\boldsymbol{M}) &= \frac{r}{\operatorname{tr}(\boldsymbol{M}^{-1})}, \\ \Phi_{\mathrm{E}}(\boldsymbol{M}) &= \eta_{r-1}(\boldsymbol{M}), \end{aligned}$$

for any $\boldsymbol{M} \in \mathcal{M}_{\boldsymbol{f},\boldsymbol{C}}$. Under particular conditions, the above criteria are indeed equivalent to their former reduced-rank versions.

Proposition 3. Under Model (1), suppose $\boldsymbol{C\beta}$ is estimable under the full OofA design $\boldsymbol{D}_m^{\mathrm{F}}$, where $\boldsymbol{C} \in \mathbb{R}^{r \times p}$ and $\operatorname{rank}(\boldsymbol{C}) = r = \operatorname{rank}(\boldsymbol{f}) \leqslant p$.

(i) There exists some $a \in (0, +\infty)$ such that, for any nonsingular OofA design measure ξ, $\Phi_0\left(\mathbf{M}_{\boldsymbol{f}}(\xi)\right) = a\Phi_0\left(\mathbf{M}_{\boldsymbol{f},\boldsymbol{C}}(\xi)\right)$, so ξ is D-optimal about $\boldsymbol{C}$ if and only if ξ is D-optimal.
(ii) Further suppose $\boldsymbol{C}\boldsymbol{C}^{\mathrm{T}} = b\mathbf{I}_r$, where $b \in (0, +\infty)$. Then, for any $u \in [-\infty, 1]$ and any nonsingular OofA design measure ξ, $\Phi_u\left(\mathbf{M}_{\boldsymbol{f}}(\xi)\right) = b\Phi_u\left(\mathbf{M}_{\boldsymbol{f},\boldsymbol{C}}(\xi)\right)$, so ξ is Φ_u-optimal about $\boldsymbol{C}$ if and only if ξ is Φ_u-optimal.

Remark 2. Proposition 3 is true for any linear model $\boldsymbol{f}$ of the form (1), not only for OofA experiments.

Proposition 3 indicates that, for preserving the general matrix mean optimality, compared to preserving the D-optimality, the matrix $\boldsymbol{C}$ has to additionally satisfy the row-orthogonality condition. This is consistent with the result of Stallings and Morgan (2015). The matrix $\boldsymbol{C}$ with mutually orthogonal rows as required in Proposition 3(ii) is not unique, and an easy way to obtain one such $\boldsymbol{C}$ is as follows. Let $\bar{\boldsymbol{F}}_f = \mathbf{F}_f(\boldsymbol{D}_m^{\mathrm{F}}) \in \mathbb{R}^{(m!)\times p}$ be the model matrix corresponding to the full OofA design. By the spectral decomposition, there exists a matrix $\boldsymbol{C} \in \mathbb{R}^{r\times p}$ such that $\boldsymbol{C}\boldsymbol{C}^{\mathrm{T}} = \mathbf{I}_r$ and $\bar{\boldsymbol{F}}_f^{\mathrm{T}}\bar{\boldsymbol{F}}_f = \boldsymbol{C}^{\mathrm{T}}\,\mathrm{diag}(a_0,\ldots,a_{r-1})\boldsymbol{C}$, where $a_0,\ldots,a_{r-1}$ are the r nonzero eigenvalues of $\bar{\boldsymbol{F}}_f^{\mathrm{T}}\bar{\boldsymbol{F}}_f$. Then, this matrix $\boldsymbol{C}$ satisfies the requirements in Proposition 3(ii). Essentially, this is exactly the procedure of the principal components regression with r principal components for the model matrix $\bar{\boldsymbol{F}}_f$. Therefore, such a $\boldsymbol{C}\boldsymbol{\beta}$ can be interpreted as the parameter vector corresponding to the r principal components. Practically, when it is hard to construct a matrix $\boldsymbol{C}$ with a satisfactory physical interpretation such that the rows of $\boldsymbol{C}$ are orthogonal to each other, one can discard the orthogonality of $\boldsymbol{C}$, and Proposition 3(ii) still guarantees the D-optimality. In addition, by the proof of Theorem 1, under a symmetric model, a COA of an enough strength has the same information matrix as that of the full OofA design, so its design measure is nonsingular. Combining the previous results, we have the following corollary for the popularly-used models introduced in Section 2.

Corollary 1. Under the CP model, sFP model or sQP model in Examples 2 and S6, for the parameter of interest $\boldsymbol{C}\boldsymbol{\beta}$ satisfying the same requirements as in Proposition 3, the design measure of a COA of strength 2 is D-optimal about $\boldsymbol{C}$. If $\boldsymbol{C}\boldsymbol{C}^{\mathrm{T}} = b\mathbf{I}_r$ with $b \in (0, +\infty)$, the design measure of a COA of strength 2 is also T-, A- and E-optimal about $\boldsymbol{C}$. The above conclusions also hold for the sTPWO, NN and sSP models in Examples 1, S4 and S7, if the COA of strength 2 is replaced by a COA of strength 4.

Example 3. Consider the sTPWO model in Example 1. We modify its intercept term from 1 to $\sqrt{2}$. This modified sTPWO model is still a 2-way symmetric model. The corresponding $\boldsymbol{C}$ in (7) now becomes $\boldsymbol{C} = \mathrm{diag}(\sqrt{2}, \mathbf{I}_{\binom{m}{2}} \otimes (1, -1))$, satisfying $\boldsymbol{C}\boldsymbol{C}^{\mathrm{T}} = 2\mathbf{I}_{1+\binom{m}{2}}$. If $\boldsymbol{\beta}$ is the parameter vector in this modified sTPWO model, then as in Example 1, $\boldsymbol{C}\boldsymbol{\beta}$ is the parameter vector in the original TPWO model. By Proposition 3 with this $\boldsymbol{C}$, we can know that any COA of strength 4 is T-, D-, A-, and E-optimal under both the modified sTPWO model and the original TPWO model. This is a generalization of Theorem 3 of Zhao, Li, and Zhao (2021).

On the other hand, Theorem 1 only provides a sufficient condition for an OofA design to have a universally optimal design measure, and it is natural to ask whether or not that condition is necessary, that is, to ask whether or not the converse proposition of Theorem 1 is true. Unfortunately, in general, the answer is negative. For example, by Theorem 1 and Proposition 2, an OofA design $\boldsymbol{D}$ has a universally optimal design measure under the sPWO model if and only if $\boldsymbol{D}$ has a D-optimal design measure under the sPWO model. By Example 1 and Proposition 3, this is equivalent to that $\boldsymbol{D}$ has a D-optimal design measure under the PWO model. By Peng, Mukerjee, and Lin (2019, p. 686) or Zhao, Lin, and Liu (2022, Theorem 4 and Corollary 2), this is equivalent to that $\boldsymbol{D}$ is an OofA-OA of strength 2. However, an OofA-OA of strength 2 need not be a COA of strength 4, so the converse of Theorem 1 does not hold under the sPWO model. Nevertheless, there are indeed models under which the converse of Theorem 1 holds.

Theorem 3. Under the CP(τ) model in Example S10 of m components with $\tau \in \{0,\ldots,m\}$, for any $u \in (-\infty, 1)$, any OofA design having a Φ_u-optimal design measure must be a COA(N, m, t), where $t = \min\{2\tau, m\}$.

By Theorem 3, the converse of Theorem 1 is true under some particular symmetric models. Thus, for example, if an OofA design has a D-optimal design measure under every τ-way symmetric model, then it has a D-optimal design measure under the CP(τ) model, so it must be a COA of strength $t = \min\{2\tau, m\}$. This implies that COAs of strength t are the unique class of OofA designs having optimal design measures under both all permutation-invariant optimality criteria and all τ-way symmetric models, simultaneously. This indicates the robustness of COAs against particular kinds of model misspecifications. For example, a COA of strength 4 is universally optimal under an arbitrary 2-way symmetric model. In contrast, although an OofA-OA of strength 2 is universally optimal under the sPWO model, its optimality is lost if one decides to use a general sTPWO model.

4. Constructions of COAs with Different Strengths

4.1. Augmentations for COAs

In this section, we propose two augmentation methods for COAs maintaining their strengths, one increasing the number of runs, and the other one increasing the numbers of both runs and components. Both methods are general and useful for constructing COAs of various strengths.

COAs of index 1 are economic, since their run sizes are minimal among all COAs of the same strength. Yang, Sun, and Xu (2021) proposed a method to construct COAs of strength 2 and more runs, based on COAs of strength 2 and index 1. We summarize and generalize their method into the following algorithm, which applies to COAs of general strengths. Its validity is immediate from Proposition 1.

Algorithm 1 (Increasing the index of a COA of index 1).

Input: (i) $\boldsymbol{D}$, a COA(N, m, t) of index 1;
(ii) $\lambda \in \{1,\ldots,(m-t)!\}$, the index of the resulting COA.

Step 1. Select arbitrary t different elements $i_0,\ldots,i_{t-1} \in \mathcal{Z}_m$, and let $\tilde{\mathcal{S}} = \{\boldsymbol{\pi} : \boldsymbol{\pi} \in \mathcal{S}_m \text{ and } \boldsymbol{\pi}(i_k) = i_k \text{ for any } k \in \mathcal{Z}_t\}$.

Step 2. Take arbitrary λ different elements $\boldsymbol{\pi}_0,\ldots,\boldsymbol{\pi}_{\lambda-1} \in \tilde{\mathcal{S}}$.

Step 3. Let

$$\hat{\boldsymbol{D}} = \begin{pmatrix} \boldsymbol{\pi}_0 \circ \boldsymbol{D} \\ \vdots \\ \boldsymbol{\pi}_{\lambda-1} \circ \boldsymbol{D} \end{pmatrix}, \quad \text{or} \quad \hat{\boldsymbol{D}} = \begin{pmatrix} \boldsymbol{D} \circ \boldsymbol{\pi}_0 \\ \vdots \\ \boldsymbol{D} \circ \boldsymbol{\pi}_{\lambda-1} \end{pmatrix}.$$

Output: $\hat{\boldsymbol{D}}$, which is a COA$(\lambda N, m, t)$ of index λ without replicated rows.

Remark 3. In Algorithm 1, when replications are allowed in the resulting design $\hat{\boldsymbol{D}}$, we can take $\boldsymbol{D}$ to be any COA(N, m, t) of any index, take λ to be any positive integer, and take the permutations $\boldsymbol{\pi}_0, \ldots, \boldsymbol{\pi}_{\lambda-1}$ in Step 2 to be any elements of $\mathcal{S}_m$.

Algorithm 1 and Remark 3 provide a method to generate COAs of higher indices, with or without replications, based on an existing COA of a smaller index. The set $\tilde{\mathcal{S}}$ in Step 1 of Algorithm 1 consists of all permutations on $\mathcal{Z}_m$ with $i_0, \ldots, i_{t-1}$ being fixed, that is, $\tilde{\mathcal{S}}$ essentially consists of all permutations on $\mathcal{Z}_m \setminus \{i_0, \ldots, i_{t-1}\}$. In practice, we can simply take $i_0, \ldots, i_{t-1}$ to be $0, \ldots, t-1$. The following example illustrates Algorithm 1.

Example 4. In Algorithm 1, we take $N = m = 4$, $t = 1$ and $\lambda = 3$, and take the initial COA$(4, 4, 1)$ to be

$$\boldsymbol{D} = \begin{pmatrix} 0 & 1 & 2 & 3 \\ 1 & 0 & 3 & 2 \\ 2 & 3 & 0 & 1 \\ 3 & 2 & 1 & 0 \end{pmatrix}.$$

In Step 1, we take $i_0 = 0$, and then $\tilde{\mathcal{S}} = \{(0, i_1, i_2, i_3) : i_1, i_2, i_3 \in \{1, 2, 3\} \text{ are distinct}\}$. In Step 2, we choose $\boldsymbol{\pi}_0 = (0, 1, 2, 3)$, $\boldsymbol{\pi}_1 = (0, 2, 3, 1)$ and $\boldsymbol{\pi}_2 = (0, 3, 1, 2)$. Then, the output $\hat{\boldsymbol{D}}$ as the right-hand side version in Step 3 is

$$\left(\begin{array}{cccc|cccc|cccc} 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 \\ 1 & 0 & 3 & 2 & 2 & 3 & 0 & 1 & 3 & 2 & 1 & 0 \\ 2 & 3 & 0 & 1 & 3 & 2 & 1 & 0 & 1 & 0 & 3 & 2 \\ 3 & 2 & 1 & 0 & 1 & 0 & 3 & 2 & 2 & 3 & 0 & 1 \end{array}\right)^{\mathrm{T}}, \tag{8}$$

where $\boldsymbol{D} \circ \boldsymbol{\pi}_0, \boldsymbol{D} \circ \boldsymbol{\pi}_1, \boldsymbol{D} \circ \boldsymbol{\pi}_2$ are separated by solid lines. Algorithm 1 guarantees that $\hat{\boldsymbol{D}}$ is a COA$(12, 4, 1)$ of index 3 without replications. In fact, the design shown in (8) is a COA$(12, 4, 2)$ of index 1, that is, the strength of the resulting COA gets increased by one compared to the initial COA.

Motivated by Example 4, one may conjecture that Algorithm 1 has the potential to improve the strength if the permutations $\boldsymbol{\pi}_0, \ldots, \boldsymbol{\pi}_{\lambda-1} \in \tilde{\mathcal{S}}$ in Step 2 are carefully selected. Unfortunately, this is not true in general. For example, all COA$(20, 5, 2)$'s and all COA$(60, 5, 3)$'s are listed in Zhao, Li, and Zhao (2021, Tables 5 and 6), from which it can be checked that any COA$(20, 5, 2)$ is not contained as a submatrix in any COA$(60, 5, 3)$. Therefore, Algorithm 1 cannot produce a COA$(60, 5, 3)$ if the initial design is a COA$(20, 5, 2)$. Nevertheless, among partial columns instead of all columns, Algorithm 1 indeed can improve the strength; please refer to Supplementary Material S3.

On the other hand, we sometimes need augment the number of components of an existing COA. For example, Huang (2021) provided a method to construct COAs of strength 2 recursively, starting from a COA of a smaller prime-power number of components. The following algorithm is a generalization of his Construction 2, inspired by the construction of Peng, Mukerjee, and Lin (2019, sec. 5) for OofA-OAs of strength 2 with an odd number of components.

Algorithm 2 (Adding a component to a COA while preserving the strength).

Input: (i) $\boldsymbol{D}$, a COA(N, m, t);
(ii) λ_Γ, an arbitrary positive integer.

Step 1. Let $\hat{\boldsymbol{D}}_0 = (\boldsymbol{D}, m\mathbf{1}_{N\times 1}) \in \mathcal{S}(N, m+1)$.

Step 2. Let $N_\Gamma = \lambda_\Gamma(m+1)$, and take an arbitrary $\boldsymbol{\Gamma} = \left(\boldsymbol{\gamma}_0^{\mathrm{T}}, \ldots, \boldsymbol{\gamma}_{N_\Gamma-1}^{\mathrm{T}}\right)^{\mathrm{T}} \in \mathcal{S}(N_\Gamma, m+1)$ such that each column of $\boldsymbol{\Gamma}$ contains the element m for exactly λ_Γ times.

Step 3. Let

$$\hat{\boldsymbol{D}} = \begin{pmatrix} \mathrm{inv}(\boldsymbol{\gamma}_0) \circ \hat{\boldsymbol{D}}_0 \\ \vdots \\ \mathrm{inv}(\boldsymbol{\gamma}_{N_\Gamma-1}) \circ \hat{\boldsymbol{D}}_0 \end{pmatrix}, \quad \text{or}$$

$$\hat{\boldsymbol{D}} = \begin{pmatrix} \hat{\boldsymbol{D}}_0 \circ \boldsymbol{\gamma}_0 \\ \vdots \\ \hat{\boldsymbol{D}}_0 \circ \boldsymbol{\gamma}_{N_\Gamma-1} \end{pmatrix}.$$

Output: $\hat{\boldsymbol{D}}$.

Theorem 4. The output $\hat{\boldsymbol{D}}$ of Algorithm 2 is a COA$(N\lambda_\Gamma(m+1), m+1, t)$. Furthermore, when $\lambda_\Gamma = 1$, $\hat{\boldsymbol{D}}$ has replicated rows if and only if $\boldsymbol{D}$ has replicated rows.

Compared with Construction 2 of Huang (2021), the above Algorithm 2 is more flexible in the matrix $\boldsymbol{\Gamma}$ in Step 2, and is applicable to COAs of general strengths. Actually, Construction 2 of Huang (2021) can be viewed as a special case of Algorithm 2 when $t = 2$ and the matrix $\boldsymbol{\Gamma}$ in Step 2 is circulant. The following example illustrates Algorithm 2.

Example 5. In Algorithm 2, we take $N = m = 3$, $t = 1$, $\lambda_\Gamma = 1$, and take the initial COA$(3, 3, 1)$ and the matrix $\boldsymbol{\Gamma}$ to be

$$\boldsymbol{D} = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 2 & 0 \\ 2 & 0 & 1 \end{pmatrix} = (\boldsymbol{\zeta}_0, \boldsymbol{\zeta}_1, \boldsymbol{\zeta}_2) \quad \text{and}$$

$$\boldsymbol{\Gamma} = \begin{pmatrix} 3 & 0 & 1 & 2 \\ 0 & 3 & 2 & 1 \\ 0 & 1 & 3 & 2 \\ 0 & 2 & 1 & 3 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\gamma}_0 \\ \boldsymbol{\gamma}_1 \\ \boldsymbol{\gamma}_2 \\ \boldsymbol{\gamma}_3 \end{pmatrix},$$

respectively. Then, $\hat{\boldsymbol{D}}_0 = (\boldsymbol{\zeta}_0, \ldots, \boldsymbol{\zeta}_3)$ in Step 1, where $\boldsymbol{\zeta}_3 = (3, 3, 3)^{\mathrm{T}}$, and the output $\hat{\boldsymbol{D}}$ as the right-hand side version in Step 3 is

$$\begin{pmatrix} \hat{\boldsymbol{D}}_0 \circ \boldsymbol{\gamma}_0 \\ \hat{\boldsymbol{D}}_0 \circ \boldsymbol{\gamma}_1 \\ \hat{\boldsymbol{D}}_0 \circ \boldsymbol{\gamma}_2 \\ \hat{\boldsymbol{D}}_0 \circ \boldsymbol{\gamma}_3 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\zeta}_3 & \boldsymbol{\zeta}_0 & \boldsymbol{\zeta}_1 & \boldsymbol{\zeta}_2 \\ \boldsymbol{\zeta}_0 & \boldsymbol{\zeta}_3 & \boldsymbol{\zeta}_2 & \boldsymbol{\zeta}_1 \\ \boldsymbol{\zeta}_0 & \boldsymbol{\zeta}_1 & \boldsymbol{\zeta}_3 & \boldsymbol{\zeta}_2 \\ \boldsymbol{\zeta}_0 & \boldsymbol{\zeta}_2 & \boldsymbol{\zeta}_1 & \boldsymbol{\zeta}_3 \end{pmatrix}$$

$$= \left(\begin{array}{ccc|ccc|ccc|ccc} 3 & 3 & 3 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 3 & 3 & 3 & 1 & 2 & 0 & 2 & 0 & 1 \\ 1 & 2 & 0 & 2 & 0 & 1 & 3 & 3 & 3 & 1 & 2 & 0 \\ 2 & 0 & 1 & 1 & 2 & 0 & 2 & 0 & 1 & 3 & 3 & 3 \end{array}\right)^{\mathrm{T}},$$

which can be obtained by replacing each symbol "i" in $\boldsymbol{\Gamma}$ with $\boldsymbol{\zeta}_i$ for each $i \in \mathcal{Z}_4$. By Theorem 4, $\hat{\boldsymbol{D}}$ is a COA$(12, 4, 1)$ of index 3 without replications. Actually, the above design $\hat{\boldsymbol{D}}$ is a

COA(12, 4, 2) of index 1. In addition, $\hat{\boldsymbol{D}}$ can be obtained from the design in (8) through interchanging the symbols "1" and "2" and permuting the rows, that is, $\hat{\boldsymbol{D}}$ is isomorphic to the design in (8).

Moreover, using Algorithm 2, we can construct a COA (180, 10, 2) of index 2, a COA(264, 12, 2) of index 2, a COA (360, 6, 4) of index 1 and a COA(1680, 7, 4) of index 2. Please refer to Supplementary Material S2 for details.

By applying Algorithm 2 recursively starting from an existing COA(N, m, t), we can obtain a series of COAs with increasing numbers of both components and runs. Most properties in Theorem 3 of Huang (2021) still hold for this generalized algorithm. To state these results formally, we need some definitions and notations. For an OofA design $\boldsymbol{D} \in \mathcal{S}(N, m)$, we define the *fraction ratio* of $\boldsymbol{D}$ to be $N/m!$, which measures how small the design $\boldsymbol{D}$ is compared to the full OofA design $\boldsymbol{D}^{\mathrm{F}}_m$. Let $A \subseteq \mathcal{Z}_m$ with Card$(A) = a$, and take a bijection $b : \mathcal{Z}_m \backslash A \to \mathcal{Z}_{m-a}$. For any $\boldsymbol{z} \in \mathcal{S}_m$, let integers $0 \leqslant i_0 < \cdots < i_{m-a-1} < m$ such that $\big(\boldsymbol{z}(i_0), \dots, \boldsymbol{z}(i_{m-a-1})\big) \in (\mathcal{Z}_m \setminus A)^{m-a}$, and define $\mathrm{drop}(\boldsymbol{z}, A) = \Big(b\big(\boldsymbol{z}(i_0)\big), \dots, b\big(\boldsymbol{z}(i_{m-a-1})\big)\Big) \in \mathcal{S}_{m-a}$. For an OofA design $\boldsymbol{D} = \big(\boldsymbol{z}_0^{\mathrm{T}}, \dots, \boldsymbol{z}_{N-1}^{\mathrm{T}}\big)^{\mathrm{T}} \in \mathcal{S}(N, m)$, define $\mathrm{drop}(\boldsymbol{D}, A) = \big(\mathrm{drop}(\boldsymbol{z}_0, A)^{\mathrm{T}}, \dots, \mathrm{drop}(\boldsymbol{z}_{N-1}, A)^{\mathrm{T}}\big)^{\mathrm{T}} \in \mathcal{S}(N, m-a)$. Then we have the following result parallel with Theorem 3 of Huang (2021).

Proposition 4. Let $\hat{\boldsymbol{D}}^{(0)} = \boldsymbol{D}$ be a COA(N, m, t) of index λ without replicated rows, and let $\hat{\boldsymbol{D}}^{(k)}$ be the output of Algorithm 2 with the input design $\hat{\boldsymbol{D}}^{(k-1)}$ and $\lambda_\Gamma = 1$ for $k = 1, 2, \dots$. Then for any $k \in \mathbb{N}$, we have:

(i) $\hat{\boldsymbol{D}}^{(k)}$ is a COA$(N\prod_{i=1}^{k}(m+i), m+k, t)$ of index $\lambda\prod_{i=1}^{k}(m-t+i)$ without replicated rows.
(ii) The fraction ratio of $\hat{\boldsymbol{D}}^{(k)}$ is the same as that of $\boldsymbol{D}$, both equaling $N/m!$.
(iii) For any $A \subseteq \{m, \dots, m+k-1\}$ with Card$(A) = a$, $\mathrm{drop}(\hat{\boldsymbol{D}}^{(k)}, A)$ is a COA$(N \cdot \prod_{i=1}^{k}(m+i), m+k-a, t)$ of index $\lambda\big(\prod_{i=1}^{k-a}(m-t+i)\big)\big(\prod_{i=1}^{a}(m+k-a+i)\big)$.

Consider the series of COAs $\hat{\boldsymbol{D}}^{(0)}, \hat{\boldsymbol{D}}^{(1)}, \dots$ in Proposition 4. Conclusion (ii) says that, from the perspective of the fraction ratio, this series of COAs are all as "small" as the starting design $\boldsymbol{D}$. On the other hand, compared with their strength t, Conclusion (i) points out that their indices increase rapidly, that is, they are becoming "larger and larger". For example, if the starting design $\boldsymbol{D}$ is a COA$(m(m-1), m, 2)$ of index 1, $\hat{\boldsymbol{D}}^{(1)}$ will be a COA$((m+1)m(m-1), m+1, 2)$ of index $(m-1)$, whose size is the same as that of a COA of strength 3 and index 1. In fact, for some special starting COA$(m(m-1), m, 2)$ and some carefully selected $\boldsymbol{\Gamma}$ in Step 2 of Algorithm 2, $\hat{\boldsymbol{D}}^{(1)}$ is indeed a COA$((m+1)m(m-1), m+1, 3)$, which is the key idea of our construction for COAs of strength 3 to be introduced in Section 4.2. Finally, Conclusion (iii) of Proposition 4 guarantees that, if some components are found irrelevant and excluded from consideration, the reduced design for the remaining components is still a COA of strength t, which benefits the analysis of the experiment.

4.2. COAs of Strength Three

To our knowledge, the first definition and instances for COAs of strength 3 are given by Zhao, Li, and Zhao (2021). For COA(60, 5, 3)'s, they found that there are only two solutions, and then tabulated them; for larger COAs of strength 3, their searching method is not suitable due to the high computational complexity. In contrast, we will propose a systematic construction method for COAs of strength 3, index 1 and prime-power-plus-one components. Then, combined with Algorithm 2 and Proposition 4, for any number of components greater than 4, our method can produce COAs of strength 3 whose numbers of runs are much less than the full OofA designs.

First, we deal with the case when the desired number of components m is a prime power plus one, that is, $m = \check{m} + 1$, with $\check{m} = b^a$, $b \in \mathbb{N}_+$ being a prime and $a \in \mathbb{N}_+$. In this case, there is a unique *Galois field* GF$(\check{m})$ of order $\check{m}$ up to isomorphism. We denote GF$(\check{m}) = \{\alpha_i : i \in \mathcal{Z}_{\check{m}}\}$, and assume that α_0 and α_1 are the identity elements for addition and multiplication (i.e., the "zero" and "one") in GF$(\check{m})$, respectively. For convenience, we may as well assume GF$(\check{m}) = \mathcal{Z}_{\check{m}}$ as a set, though the operations on GF$(\check{m})$ can be quite different from those on $\mathcal{Z}_{\check{m}} \subseteq \mathbb{R}$. For elements in $\mathcal{Z}_{\check{m}}$, when we emphasize they are elements of GF$(\check{m})$, the operations between them are on the field GF$(\check{m})$, and otherwise, the operations are on $\mathcal{Z}_{\check{m}} \subseteq \mathbb{R}$ as usual. This should make no ambiguity. Our construction method for the COA of m components, strength 3 and index 1 is as follows.

Algorithm 3 (Construction for COAs of strength 3 and index 1).

Input: m, the number of components, which is a prime power plus one.

Step 1. Let $\check{m} = m - 1$ and $\check{N} = \check{m}(\check{m}-1)$. Generate a matrix $\check{\boldsymbol{D}} \in \mathrm{GF}(\check{m})^{\check{N}\times\check{m}}$ such that for any $i, j \in \mathcal{Z}_{\check{m}}$ and $k \in \{0, \dots, \check{m}-2\}$, the $(k\check{m}+i, j)$th entry of $\check{\boldsymbol{D}}$ is $\check{\boldsymbol{D}}(k\check{m}+i, j) = \alpha_i + \alpha_{k+1}\alpha_j$.

Step 2. Let $\boldsymbol{D}_0 = \Big(\check{\boldsymbol{D}}, \check{m}\boldsymbol{1}_{\check{N}\times 1}\Big) \in \mathcal{S}(\check{N}, m)$.

Step 3. Construct a matrix $\boldsymbol{\Gamma} \in \mathcal{S}(m, m)$ such that for any $i, j \in \mathcal{Z}_m$, the (i, j)th entry of $\boldsymbol{\Gamma}$ is

$$\boldsymbol{\Gamma}(i,j) = \begin{cases} \check{m}, & i = j; \\ \alpha_{j-1}, & i = 0 \text{ and } j \geqslant 1; \\ \alpha_0, & i \geqslant 1 \text{ and } j = 0; \\ \alpha_{j-1}^{-1}, & i = 1 \text{ and } j \geqslant 2; \\ \alpha_1, & i \geqslant 2 \text{ and } j = 1; \\ \alpha_{i-1}(\alpha_{i-1} - \alpha_{j-1})^{-1}, & i \geqslant 2 \text{ and } j \geqslant 2 \text{ and } i \neq j. \end{cases}$$

Step 4. Denote $\boldsymbol{\Gamma} = \big(\boldsymbol{\gamma}_0^{\mathrm{T}}, \dots, \boldsymbol{\gamma}_{m-1}^{\mathrm{T}}\big)^{\mathrm{T}}$, and let

$$\boldsymbol{D} = \begin{pmatrix} \boldsymbol{D}_0 \circ \boldsymbol{\gamma}_0 \\ \vdots \\ \boldsymbol{D}_0 \circ \boldsymbol{\gamma}_{m-1} \end{pmatrix}.$$

Output: $\boldsymbol{D}$.

The above algorithm is a special case of Algorithm 2, with the input design being $\check{\boldsymbol{D}}$ in Step 1 of Algorithm 3, $\lambda_\Gamma = 1$, and the particular $\boldsymbol{\Gamma}$ in Step 3 of Algorithm 3. In fact, $\check{\boldsymbol{D}}$ in Step 1 of Algorithm 3 is a COA$(\check{N}, \check{m}, 2)$ of index 1 obtained by Algorithm 1 of Stokes and Xu (2022); please see Supplementary Material S4 for more properties of $\check{\boldsymbol{D}}$. The validity of Algorithm 3 is guaranteed by the following theorem.

Theorem 5. The output $\boldsymbol{D}$ of Algorithm 3 is a COA$(P_m^3, m, 3)$ of index 1.

Theorem 5 guarantees that COAs of prime-power-plus-one components, strength 3 and index 1 exist, and they can be constructed via Algorithm 3. For COAs of prime-power-plus-one components, strength 3 and higher indices, we can apply Algorithm 1 to the output of Algorithm 3. An example illustrating Algorithm 3 is provided in Supplementary Material S2.

On the other hand, when the desired number of components $m \geqslant 7$ is not a prime power plus one, the corresponding COA of strength 3 cannot be obtained from Algorithm 3 directly. For such a case, one can first find the largest integer m_0 which is a prime power plus one such that $6 \leqslant m_0 < m$, then construct a COA of m_0 components and strength 3, and recursively apply Algorithm 2 until the resulting COA has m components.

4.3. COAs of Higher Strengths

Practically, the number of runs of a COA of strength $t \geqslant 4$ may be too large to afford. However, theoretically, it is still worthwhile to investigate COAs of strengths 4 and higher. The construction for COAs of such high strengths is quite difficult and the results are very limited, since we have not found any powerful tools, and meanwhile there are few inspiring instances.

For COAs of strength 4, we try to construct them by applying Algorithm 2, with appropriate matrices $\boldsymbol{\Gamma}$ in Step 2 obtained by computer searches, to the COAs of strength 3 constructed by Algorithm 3. As a result, we obtain a COA$(360, 6, 4)$ of index 1 and a COA$(1680, 7, 4)$ of index 2. Please refer to Supplementary Material S2 for details. Interestingly, for that COA$(360, 6, 4)$, the set of its rows is the alternating group on $\mathcal{Z}_m$, denoted by $\mathcal{A}_m$, with $m = 6$. In fact, this is a general phenomenon.

Theorem 6. For any integer $m \geqslant 3$, an OofA design $\boldsymbol{D}$ is a COA$(m!/2, m, m-2)$ of index 1 if and only if the set of rows of $\boldsymbol{D}$ is either $\mathcal{A}_m$ or $\mathcal{S}_m \setminus \mathcal{A}_m$.

Theorem 6 says that, for $m \geqslant 3$, there are exactly two COAs of m components, strength $m-2$ and index 1, up to row permutations. For example, there are exactly two COA$(3, 3, 1)$'s, two COA$(12, 4, 2)$'s, two COA$(60, 5, 3)$'s and two COA$(360, 6, 4)$'s. This confirms and generalizes the findings of Zhao, Li, and Zhao (2021, Corollaries 1 and 5).

For convenience, we summarize some known construction results for COAs of as small as possible indices in Table 2. For the rows in Table 2 with a "$*$" after their indices, the constructed COAs achieve the minimum indices, while for the other rows, the constructed COAs only provide upper bounds for the corresponding minimum indices and the exact values of their minimum indices need further research.

Table 2. Some known COAs of m components, strengths t and as small as possible indices λ.

t	m	λ	Constructions
1	At least 2	$1*$	† Any Latin square
2	Prime power	$1*$	Algo. 2 of Yang, Sun, and Xu (2021)
2	5	$1*$	† Zhao, Li, and Zhao (2021, Table 5)
2	Non "prime power"	By Prop. 4	Algo. 2 of Yang, Sun, and Xu (2021) combined with Algo. 2
2	6	$2*$	Zhao, Li, and Zhao (2021)
2	10	$2*$	Example S12
2	12	2	Example S13
3	Prime power plus one	$1*$	Algo. 3
3	Non "prime power plus one"	By Prop. 4	Algo. 3 combined with Algo. 2
4	7	$2*$	Example S14
$m-2$	At least 3	$1*$	† Theorem 6
m	At least 2	$1*$	† Full OofA design

NOTE: Those marked with "$*$" after their indices achieve the minimum indices. The constructions marked with "†" can generate all COA$(\lambda P_m^t, m, t)$'s in respective cases. "Algo." stands for "Algorithm" and "Prop." stands for "Proposition".

5. Concluding Remarks

In this article, we propose a broad class of linear regression models for OofA experiments, called the symmetric linear models, which includes almost all popularly-used linear models for OofA experiments in the sense of equivalence, and includes infinitely many new models as well. Under the symmetric linear models, we find that COAs have universally optimal design measures, and for some special cases, COAs are the only designs with universally optimal design measures. These results reveal the efficiency and robustness of COAs. As for the constructions of COAs, we generalize the existing methods, and creatively propose a systematic construction method for COAs of strength 3 and index 1. We also provide some particular constructions of COAs of strengths 2, 4 and higher. Moreover, the numerical results in Supplementary Material S5 justify our theoretical results and further indicate that COAs may have many other appealing properties not covered by our theoretical results. Therefore, in practice, these results will promote the use of COAs.

However, there are still some unsolved issues for COAs, say for example, (i) With given number of components m and strength t, how to determine the minimum index λ^* such that a COA$(\lambda^* P_m^t, m, t)$ exists? (ii) How to construct and classify all COA(N, m, t)'s if there exists a COA(N, m, t)? These issues still need further study, and we hope some of them can be solved in the future.

Supplementary Materials

The supplementary materials include some additional examples and theories, numerical comparisons, and the proofs of the main theoretical results. The C++ source codes to generate the numerical results in Supplementary Material S5 and a computer program written in C++ to generate the COAs in Table 2 are also provided.

Acknowledgments

The authors thank Dr. Xiangshun Kong for his help on Proposition 2. The authors also thank Editor Dylan Small, an associate editor and five referees for their valuable comments and suggestions. The first two authors contributed equally to this work.

Disclosure Statement

The authors report there are no competing interests to declare.

Funding

This work was supported by the National Nature Science Foundation of China (Grant Nos. 12131001 and 12371260).

References

Chen, J., Han, X., Lin, D. K. J., Yang, L., and Zhou, Y. (2023), "On Ordering Problems: A Statistical Approach," *Statistica Sinica*, 33, 1903–1922. [1,4]

Chen, J., Mukerjee, R., and Lin, D. K. J. (2020), "Construction of Optimal Fractional Order-of-Addition Designs via Block Designs," *Statistics & Probability Letters*, 161, 108728. [2]

Fisher, R. A. (1971), *The Design of Experiments* (9th ed.), New York: Hafner Press. [1]

Huang, H. (2021), "Construction of Component Orthogonal Arrays with Any Number of Components," *Journal of Statistical Planning and Inference*, 213, 72–79. [1,2,8,9]

Huang, J. W., and Phoa, F. K. H. (2024), "Complete Consecutive Order-Pairing (CCOP) Design and its Distance-based Linear Model: Design Construction and Analysis for Order-of-Addition (OofA) Experiments," *Statistica Sinica*, preprint. DOI:10.5705/ss.202023.0357 [3]

Kiefer, J. (1975), "Construction and Optimality of Generalized Youden Designs," in *A Survey of Statistical Design and Linear Models*, eds. J. N. Srivastava, pp. 333–353, Amsterdam: North-Holland. [5]

Kong, X., Yuan, M., and Zheng, W. (2021), "Approximate and Exact Designs for Total Effects," *The Annals of Statistics*, 49, 1594–1625. [5]

Lin, D. K. J., and Peng, J. (2019), "Order-of-Addition Experiments: A Review and Some New Thoughts," *Quality Engineering*, 31, 49–59. [1,4]

Mee, R. W. (2020), "Order-of-Addition Modeling," *Statistica Sinica*, 30, 1543–1559. [1,3,4]

Mee, R. W. (2024), "Synthesis of Order-of-Addition Models," *Statistica Sinica*, 34, 589–610. [1,3,4]

Peng, J., Mukerjee, R., and Lin, D. K. J. (2019), "Design of Order-of-Addition Experiments," *Biometrika*, 106, 683–694. [1,2,4,5,7,8]

Piepho, H. P., and Williams, E. R. (2021), "Regression Models for Order-of-Addition Experiments," *Biometrical Journal*, 63, 1673–1687. [3,4]

Pukelsheim, F. (2006), *Optimal Design of Experiments*, Philadelphia: SIAM. [5]

Rios, N., Winker, P., and Lin, D. K. J. (2022), "TA Algorithms for D-Optimal OofA Mixture Designs," *Computational Statistics & Data Analysis*, 168, 107411. [1]

Stallings, J. W., and Morgan, J. P. (2015), "General Weighted Optimality of Designed Experiments," *Biometrika*, 102, 925–935. [7]

Stokes, Z., and Xu, H. (2022), "A Position-based Approach for Design and Analysis of Order-of-Addition Experiments," *Statistica Sinica*, 32, 1467–1488. [1,3,4,10]

Van Nostrand, R. C. (1995), "Design of Experiments Where the Order of Addition is Important," in *ASA Proceeding of the Section on Physical and Engineering Sciences*, pp. 155–160, Alexandria, VA: American Statistical Association. [1,3,4]

Voelkel, J. G. (2019), "The Design of Order-of-Addition Experiments," *Journal of Quality Technology*, 51, 230–241. [1]

Xiao, Q., Wang, Y., Mandal, A., and Deng, X. (2024), "Modeling and Active Learning for Experiments with Quantitative-Sequence Factors," *Journal of the American Statistical Association*, 119, 407–421. [1,3]

Xiao, Q., and Xu, H. (2021), "A Mapping-based Universal Kriging Model for Order-of-Addition Experiments in Drug Combination Studies," *Computational Statistics & Data Analysis*, 157, 107155. [3]

Yang, J. F., Sun, F., and Xu, H. (2021), "A Component-Position Model, Analysis and Design for Order-of-Addition Experiments," *Technometrics*, 63, 212–224. [1,2,3,4,7,10]

Yang, L., Zhou, Y., Fu, H., Liu, M. Q., and Zheng, W. (2024), "Fast Approximation of the Shapley Values based on Order-of-Addition Experimental Designs," *Journal of the American Statistical Association*, 119, 2294–2304. [1]

Yang, L., Zhou, Y., and Liu, M. Q. (2023), "Ordering Factorial Experiments," *Journal of the Royal Statistical Society*, Series B, 85, 869–885. [1]

Zhao, Y., Li, Z., and Zhao, S. (2021), "A New Method of Finding Component Orthogonal Arrays for Order-of-Addition Experiments," *Metrika*, 84, 805–824. [1,2,4,7,8,9,10]

Zhao, Y., Lin, D. K. J., and Liu, M. Q. (2022), "Optimal Designs for Order-of-Addition Experiments," *Computational Statistics & Data Analysis*, 165, 107320. [1,7]