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Models for Order-of-Addition Screening Experiments

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Abstract: In many physical and engineering experiments, the order in which a process is executed or components are added can have a marked impact on the response. Due to constraints on resources or feasibility, there are situations where only a subset of the components can be administered in practice and experimenters encounter a complicated task with the selection of components and the corresponding best order. We present a series of models for such order-of-addition screening experiments and study their properties. We develop theoretical results on the corresponding optimal designs and illustrate these models on job scheduling problems with job rejection penalties.

Key words and phrases: Component screening model, experimental design, job scheduling, linear model, order-of-addition experiment.

1. Introduction

Order-of-addition experiments, as the name suggests, aim to study the effects caused by order arrangement of components. One of the main purposes

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of such experiments is to optimize the response by changing the order of components. There are a wide range of applications for order-of-addition experiments, such as drug combination studies (Wang et al., 2020; Xiao and Xu, 2021; Huang et al., 2023), job scheduling problems (Lin and Peng, 2019; Lin and Rios, 2025), teamwork races (Perera et al., 2016), income distribution problems (Yang et al., 2024), and many others. To describe the response surface, two different ways to explain the effects of component order have been developed. Firstly, Van Nostrand (1995) proposed the pairwise-order (PWO) model to describe the effects of relative positions of components. Lin and Peng (2019) and Mee (2020) further generalized the model to describe the relative positions of more than two components. Under the PWO model, a good design can be an order-of-addition orthogonal array (Voelkel, 2019; Chen et al., 2020; Schoen and Mee, 2023) or equivalently, an optimal design (Peng et al., 2019; Zhao et al., 2022). Secondly, Yang et al. (2021) proposed the component-position (CP) model by considering the absolute positions of components and the corresponding optimal designs, namely component orthogonal arrays. Stokes and Xu (2022) and Xiao and Xu (2021) regarded the application time of components as a quantitative factor and further proposed the quantitative CP models. Mee (2024) renamed the CP model as the nominal component-position (NCP)

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model to distinguish it from the quantitative CP models. On the other hand, Yang et al. (2023) generalized the original CP model with interactions. These designs and models help experimenters to better understand how to arrange the application order of components such that the response is desirable, and explain why it works. Readers can refer to Lin and Peng (2019), Mee (2024) and Lin and Rios (2025) for detailed reviews. Among many others, some recent developments include Stokes et al. (2024); Xiao et al. (2024); Yang et al. (2024); Liu et al. (2025); Rios and Lin (2025); Huang and Yang (2025); Zhao et al. (2025); Zheng and Rios (2025); Huang and Phoa (2026).

While these approaches effectively capture order effects, the original framework may be inadequate when certain constraints are imposed on the order arrangement. For instance, the number of components considered may be larger than the number of available positions in a run. Issues may arise where an experimenter considers many drugs but intends to use only a portion of them due to restriction in practice (Stokes and Xu, 2024). In job scheduling problems, limitations on the affordable number of jobs due to a tight budget could also impact the applicability of the original framework. Likewise, the number of available members in a baseball team is larger than the number of batters in a batting order during a baseball

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game. The constraint here is that the number of components in an order is smaller than the total number of components considered. Many cases in the real world, including but not limited to all the examples above, show that screening components from a large potential candidate set is important. This paper aims at addressing such problems. The focus is on selecting a subset of components while investigating the order effects of the components selected. To the best of our knowledge, Stokes and Xu (2024) appears to be the only primary literature that considered the component screening problem in order-of-addition experiments while Khan et al. (2025) applied their framework for identifying optimal drug combination therapies to eliminate intracellular bacteria infections by selecting three drugs from total five drugs and administering them sequentially.

To address this objective, we adopt the order-of-addition component screening framework outlined in Stokes and Xu (2024). In this context, the term "screening" denotes the process of selecting components, and the number of components in a single experimental run or treatment is smaller than the total number of components. This situation implies that not all components are essential for the final application, but rather, they are potential candidates for forming an effective treatment. Stokes and Xu (2024) extended the original order-of-addition effects by including an extra level

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to indicate whether a component is present in a treatment. On this basis, we further tackle the effects of the component order and the component selection simultaneously by proposing a series of new models with component indicators. We study the relationship between the basic order-of-addition component screening models in Stokes and Xu (2024) and our new models, derive the structures of the information matrices for full designs as well as some existing designs, and summarize the conditions of D-optimal designs. In the numerical study, we show that, under different job scheduling simulators, the models with component indicators have better performances on model goodness of fit and prediction than those without component indicators.

The paper is organized as follows. Section 2 reviews the existing models, associated designs, and background of optimal designs. Section 3 describes our new models and their statistical properties under the full design. Section 4 studies smaller and efficient component screening designs. Section 5 presents the simulation results under a job scheduling scenario with rejection penalties. Section 6 gives some concluding remarks. All proofs are provided in the Supplementary Material.

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2. Preliminaries

Suppose that there are total m components, denoted as $1, \ldots, m$, but only $q < m$ positions are available. The problem is to choose q components from the total m components and order them. As in Stokes and Xu (2024), we assume that q is fixed and pre-determined by the physical limitations of the application and $3 \leq q < m$. The full design consists of $\binom{m}{q} q! = m!/(m-q)!$ runs, where each run corresponds to q distinct components in a certain order. Throughout the paper, we denote a run as $\boldsymbol{x} = (x_1, \ldots, x_q)$, where $x_1, \ldots, x_q$ represent q distinct components, taking values from 1 to m.

2.1 PWO Model and its Screening Version

In accordance with the pseudo-factor methodology initially introduced by Van Nostrand (1995) and Voelkel (2019) and extended by Peng et al. (2019), we review the framework of the PWO model. This framework pertains to situations where there exist m distinct components, such as drugs or reactants. The relative position between components i and j is treated as the PWO factor

$$Z_{i,j}(\boldsymbol{x}) = \begin{cases} 1, & \text{if component } i \text{ is applied before component } j, \\ -1, & \text{if component } j \text{ is applied before component } i. \end{cases}$$

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The PWO model is

$$y = \beta_0 + \sum_{1 \le i < j \le m} Z_{i,j}(\boldsymbol{x})\gamma_{ij} + \epsilon, \tag{2.1}$$

where y is the response, β_0 is the intercept, γ_{ij} is the PWO effect, and ϵ is a random error. The PWO model has $1 + m(m-1)/2$ parameters.

Consequently, this approach yields a model matrix equivalent to the main effect model of a two-level factorial design. A full PWO design is essentially defined as a full factorial design with the exclusion of infeasible level combinations and a fractional PWO design constitutes a subset of a full PWO design. The infeasible level combinations are those that do not satisfy a transition law in relative positions. For example, $Z_{1,2} = 1$ and $Z_{2,3} = 1$ uniquely determine the order 123, and $Z_{1,3} = -1$ is infeasible given $(Z_{1,2}, Z_{2,3}) = (1, 1)$, making the situation different from the traditional factorial design. With this definition, the design and analysis for order-of-addition design problems are converted to two-level factorial design and analysis problems with constraints, and many researches based on this concept have been developed. The D-optimal designs for the PWO model are the order-of-addition orthogonal arrays (OofA-OA's), and a design $\boldsymbol{\xi} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ is an OofA-OA of strength 2 if for any two columns

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in

$$\begin{pmatrix} Z_{1,2}(\boldsymbol{x}_1) & \cdots & Z_{m-1,m}(\boldsymbol{x}_1) \\ \vdots & \ddots & \vdots \\ Z_{1,2}(\boldsymbol{x}_n) & \cdots & Z_{m-1,m}(\boldsymbol{x}_n) \end{pmatrix},$$

the frequencies of $(1,1), (-1,1), (1,-1), (-1,-1)$ are proportional to that of the full design.

The screening version of the PWO model, proposed by Stokes and Xu (2024), extends the definition of $Z_{i,j}(\boldsymbol{x})$ to be

$$Z_{i,j}(\boldsymbol{x}) = \begin{cases} 1, & \text{if component } i \text{ is applied before component } j, \\ -1, & \text{if component } j \text{ is applied before component } i, \\ 0, & \text{if either component } i \text{ or } j \text{ is missing.} \end{cases} \quad (2.2)$$

With the modified PWO factor (2.2), the PWO model remains the same as (2.1).

2.2 NCP Model and its Screening Version

Yang et al. (2021) introduced the NCP model to investigate the impact of components and positions in order-of-addition problems. This perspective posits that the specific placement of components within a sequence holds significant relevance. Yang et al. (2021) designated the component-position factors as

$$X_i^{(j)}(\boldsymbol{x}) = \begin{cases} 1, & \text{if component } i \text{ is placed at position } j, \\ 0, & \text{otherwise.} \end{cases} \quad (2.3)$$

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The NCP model is

$$y = \beta_0 + \sum_{i=1}^{m} \sum_{j=1}^{m} X_i^{(j)}(\boldsymbol{x})\beta_{ij} + \epsilon, \tag{2.4}$$

where β_{ij} is the effect of component i when it is placed at position j. The NCP model is over-parameterized because for every $\boldsymbol{x}$, $\sum_{i=1}^{m} X_i^{(j)}(\boldsymbol{x}) = 1$ for each j and $\sum_{j=1}^{m} X_i^{(j)}(\boldsymbol{x}) = 1$ for each i. There are $2m-1$ independent constraints and the number of identifiable parameters in the NCP model (2.4) is $1 + (m-1)^2$.

Yang et al. (2021) also proposed its corresponding optimal design, the component orthogonal array (COA). An $n \times m$ design is called a COA(n, m) if (i) each row is a permutation of $\{1, 2, \ldots, m\}$ and (ii) for any two columns, all (i, j) combinations for $1 \leq i \neq j \leq m$ appear the same number of times.

In the screening case, not all components are used in each run. When $q < m$, because only q positions are available, an identifiable NCP model (Stokes and Xu, 2024) is

$$y = \beta_0 + \sum_{i=1}^{m-1} \sum_{j=1}^{q} X_i^{(j)}(\boldsymbol{x})\beta_{ij} + \epsilon, \tag{2.5}$$

which has $1 + (m-1)q$ parameters.

2.3 Quantitative CP Models

Like the NCP model, the quantitative CP models introduced by Stokes

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and Xu (2022) incorporate absolute component positions. However, rather than using component-position indicators, they treated these positions as quantitative time points representing when each component is applied.

Let $\boldsymbol{x} = (x_1, \dots, x_m)$ be a permutation of the m components $\{1, 2, \dots, m\}$. For $i = 1, \dots, m$, define $b_i(\boldsymbol{x}) = k$ if $x_k = i$. The vector $b(\boldsymbol{x}) = (b_1(\boldsymbol{x}), \dots, b_m(\boldsymbol{x}))$ records the positions when each component appears in $\boldsymbol{x}$. Based on this, Stokes and Xu (2022) defined three quantitative CP models as follows:

$$y = \beta_0 + \sum_{i=1}^{m-1} p_1(b_i(\boldsymbol{x}))\beta_i + \epsilon, \tag{2.6}$$

$$y = \beta_0 + \sum_{i=1}^{m-1} p_1(b_i(\boldsymbol{x}))\beta_i + \sum_{i=1}^{m-1} p_2(b_i(\boldsymbol{x}))\beta_{ii} + \epsilon, \tag{2.7}$$

$$\begin{aligned} y = {} & \beta_0 + \sum_{i=1}^{m-1} p_1(b_i(\boldsymbol{x}))\beta_i + \sum_{i=1}^{m-2} p_2(b_i(\boldsymbol{x}))\beta_{ii} \\ & + \sum_{i=1}^{m-2} \sum_{j=i+1}^{m-1} p_1(b_i(\boldsymbol{x}))p_1(b_j(\boldsymbol{x}))\beta_{ij} + \epsilon, \end{aligned} \tag{2.8}$$

where $p_1(x) = c_1(x - \frac{m+1}{2})$ and $p_2(x) = c_2[(x - \frac{m+1}{2})^2 - (\frac{m^2-1}{12})]$ are orthogonal polynomials of degrees 1 and 2, respectively, and c_1 and c_2 are normalizing constants. Models (2.6), (2.7) and (2.8) are called the first-order, pure quadratic and second-order CP models, and abbreviated as the FOCP, QCP and SOCP models accordingly.

In contrast to the PWO and NCP models, the quantitative CP models have not been extended to the component screening problems yet. We will

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extend these quantitative CP models in Section 3.2.

2.4 Optimal Design Background

For an n-run design $\boldsymbol{\xi} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ and the corresponding linear model $y = f(\boldsymbol{x})^T\beta + \epsilon$, the per-run information matrix is defined as

$$M(\boldsymbol{\xi}) = \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{x}_i)f(\boldsymbol{x}_i)^T = \frac{1}{n}\boldsymbol{X}^T\boldsymbol{X},$$

where $\boldsymbol{X} = (f(\boldsymbol{x}_1), \cdots, f(\boldsymbol{x}_n))^T$ is the model matrix. With reference to the models introduced above, we have $f(\boldsymbol{x}) = (1, Z_{1,2}(\boldsymbol{x}), \ldots, Z_{m-1,m}(\boldsymbol{x}))^T$ for the PWO model (2.1) and $f(\boldsymbol{x}) = (1, X_1^{(1)}(\boldsymbol{x}), \ldots, X_q^{(m-1)}(\boldsymbol{x}))^T$ for the NCP model (2.5).

The D-optimal design maximizes the determinant of $M(\boldsymbol{\xi})$, promoting overall precision in all parameter estimations. The general equivalence theorem (Kiefer and Wolfowitz, 1960) states that a design $\boldsymbol{\xi}$ is D-optimal if and only if for all $\boldsymbol{x}$,

$$f(\boldsymbol{x})^T M(\boldsymbol{\xi})^{-1} f(\boldsymbol{x}) \leq p, \tag{2.9}$$

and the equality holds for every $\boldsymbol{x} \in \boldsymbol{\xi}$, where p is the number of columns of the information matrix $M(\boldsymbol{\xi})$. The general equivalence theorem implies that a D-optimal design is also a G-optimal design (Wong, 1994), where the G-optimal design minimizes the maximum variance of the predicted values

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across the entire experimental design space.

3. Order-of-Addition Screening Models

3.1 New Component Indicator Models

To address the influences from absence/presence of components, we define *component indicators* to represent which components are included in a run. For $k = 1, \ldots, m$, define

$$S_k(\boldsymbol{x}) = \begin{cases} 1, & \text{if component } k \text{ is present in } \boldsymbol{x}, \\ 0, & \text{otherwise.} \end{cases} \tag{3.1}$$

Since every run has exact q positions, there is a constraint $\sum_{k=1}^{m} S_k(\boldsymbol{x}) = q$ for any $\boldsymbol{x}$.

We can add $m-1$ component indicators to the PWO model (2.1), and get

$$y = \beta_0 + \sum_{k=1}^{m-1} S_k(\boldsymbol{x})\alpha_k + \sum_{1 \le i < j \le m} Z_{i,j}(\boldsymbol{x})\gamma_{ij} + \epsilon, \tag{3.2}$$

where α_k is the effect of component k. Model (3.2) is named as the PWOi model.

Since the full design contains all permutations of any q components, for all $\boldsymbol{x}$ in the full design satisfying $S_k(\boldsymbol{x}) = 1$, the number of times $Z_{i,j}(\boldsymbol{x}) = 1$ is equal to the number of times $Z_{i,j}(\boldsymbol{x}) = -1$. We have the following result.

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Lemma 1. *The PWO factors* $Z_{i,j}(\boldsymbol{x})$*'s are orthogonal to the component indicators* $S_k(\boldsymbol{x})$*'s for all* $i \neq j$ *under the full design.*

Stokes and Xu (2024) have proved that the full design is D-optimal under the PWO model when $q < m$. We further obtain the corresponding optimality result for the PWOi model.

Theorem 1. *The full design is D-optimal under the PWOi model* (3.2)*.*

On the other hand, by the definitions, $S_i(\boldsymbol{x}) = \sum_{j=1}^{m} X_i^{(j)}(\boldsymbol{x})$ for any $\boldsymbol{x}$; that is, a component indicator is the sum of its corresponding NCP variables. In other words, the information of the component indicators is already explained by the NCP model; therefore, there is no need to add the component indicators to the NCP model.

3.2 Quantitative CP Screening Models

The quantitative CP models cannot be directly used for component screening experiments because not all components appear in each run when $q < m$. To extend these models, we first modify the definition of the position function $b_i(\boldsymbol{x})$. For $i = 1, \ldots, m$ and a run $\boldsymbol{x} = (x_1, \ldots, x_q)$ with $q < m$, define

$$b_i(\boldsymbol{x}) = \begin{cases} k, & \text{if } x_k = i, \\ 0, & \text{otherwise,} \end{cases} \tag{3.3}$$

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where $b_i(\boldsymbol{x}) = 0$ implies that the component i does not appear in the run $\boldsymbol{x}$. For example, when $m = 5$ and $q = 3$, for $\boldsymbol{x} = (3, 1, 4)$, the position vector is $b(\boldsymbol{x}) = (b_1(\boldsymbol{x}), \ldots, b_5(\boldsymbol{x})) = (2, 0, 1, 3, 0)$.

With the added level $b_i(\boldsymbol{x}) = 0$, we further modify the corresponding orthogonal polynomials as follows:

$$p_1(x) = \begin{cases} c_1(x - \frac{q+1}{2}), & \text{if } x > 0, \\ 0, & \text{if } x = 0, \end{cases} \tag{3.4}$$

and

$$p_2(x) = \begin{cases} c_2[(x - \frac{q+1}{2})^2 - (\frac{q^2-1}{12})], & \text{if } x > 0, \\ 0, & \text{if } x = 0, \end{cases} \tag{3.5}$$

where the normalization constants c_1 and c_2 satisfy

$$\sum_{j=1}^{q} p_1(j) = \sum_{j=1}^{q} p_2(j) = 0 \text{ and } \sum_{j=1}^{q} p_1(j)^2 = \sum_{j=1}^{q} p_2(j)^2 = q. \tag{3.6}$$

With these modifications, the FOCP and QCP models remain the same as (2.6) and (2.7), while the SOCP model becomes

$$\begin{aligned} y = \beta_0 &+ \sum_{i=1}^{m-1} p_1(b_i(\boldsymbol{x}))\beta_i + \sum_{i=1}^{m-1} p_2(b_i(\boldsymbol{x}))\beta_{ii} \\ &+ \sum_{i=1}^{m-2} \sum_{j=i+1}^{m} p_1(b_i(\boldsymbol{x}))p_1(b_j(\boldsymbol{x}))\beta_{ij} + \epsilon. \end{aligned} \tag{3.7}$$

There is a key difference between the original SOCP model (2.8) and our extended version (3.7). The former satisfies the relationship that $(p_1(b_i(\boldsymbol{x}))/c_1)^2 - p_2(b_i(\boldsymbol{x}))/c_2$ is a constant for any $\boldsymbol{x}$ when $q = m$. This does not hold for the

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latter because $q < m$. Therefore, the number of estimable parameters in our extended model is $(m+4)(m-1)/2$ while that of the original SOCP model is $(m+2)(m-1)/2$. The extended SOCP model accommodates $(m-1)$ more parameters than the original SOCP model. As the following lemma shows, these additional $m-1$ parameters provide exactly the same information as the component indicators.

Lemma 2. *The component indicators are spanned by the column space of the SOCP model.*

By Lemma 2, there is no need to add the component indicators to the SOCP model (3.7). Thus, we consider only adding the component indicators to the FOCP and QCP models and get

$$y = \beta_0 + \sum_{k=1}^{m-1} S_k(\boldsymbol{x})\alpha_k + \sum_{i=1}^{m-1} p_1(b_i(\boldsymbol{x}))\beta_i + \epsilon, \quad (3.8)$$

$$y = \beta_0 + \sum_{k=1}^{m-1} S_k(\boldsymbol{x})\alpha_k + \sum_{i=1}^{m-1} p_1(b_i(\boldsymbol{x}))\beta_i + \sum_{i=1}^{m-1} p_2(b_i(\boldsymbol{x}))\beta_{ii} + \epsilon, \quad (3.9)$$

which are named as the FOCPi and QCPi models, respectively.

Lemma 3. *The factors $p_1(b_i(\boldsymbol{x}))$'s and $p_2(b_i(\boldsymbol{x}))$'s are orthogonal to the component indicators $S_k(\boldsymbol{x})$'s under the full design.*

Lemma 3 implies that the FOCPi and QCPi models are identifiable and adding component indicators to the FOCP and QCP models are meaningful.

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In addition, it is possible to construct a good design such that the estimators of quantitative CP effects β_i's, β_{ii}'s and β_{ij}'s are independent to that of the component indicator effect α_k.

Example 1. Consider one of the job scheduling problems described in Stokes and Xu (2024). The true model that generates the response Y will be explained in Section 5. Table 1 presents the full design and responses for the case $m = 4$ and $q = 3$. For a run $\boldsymbol{x} = (x_1, x_2, x_3)$, the corresponding vector $b(\boldsymbol{x}) = (b_1, b_2, b_3, b_4)$ records the positions of the components. We compare all models fitted to this data in terms of the number of identifiable parameters (p), R^2 and adjusted R^2 in Table 2. As we can see, the three models (PWOi, FOCPi and QCPi) with component indicators improved the goodness-of-fit results comparing to the corresponding models (PWO, FOCP and QCP) without component indicators. As $q = 3$, the NCP and QCPi models are equivalent; therefore, the two models have identical R^2 values and adjusted R^2 values in Table 2. The SOCP model has the largest number of parameters and fits the data best.

The next two theorems describe the D-optimality of the full design under various quantitative CP models.

Theorem 2. *(i) When $3 \leq q < m$, the full design is D-optimal under the FOCP model* (2.6) *and the QCP model* (2.7).

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Table 1: Design and responses for a four-component experiment.

Run	x_1	x_2	x_3	b_1	b_2	b_3	b_4	Y
1	1	2	3	1	2	3	0	727
2	1	2	4	1	2	0	3	1219
3	1	3	2	1	3	2	0	893
4	1	3	4	1	0	2	3	1324
5	1	4	2	1	3	0	2	889
6	1	4	3	1	0	3	2	780
7	2	1	3	2	1	3	0	995
8	2	1	4	2	1	0	3	1487
9	2	3	1	3	1	2	0	1769
10	2	3	4	0	1	2	3	1757
11	2	4	1	3	1	0	2	1669
12	2	4	3	0	1	3	2	1101
13	3	1	2	2	3	1	0	1307
14	3	1	4	2	0	1	3	1738
15	3	2	1	3	2	1	0	1887
16	3	2	4	0	2	1	3	1875
17	3	4	1	3	0	1	2	1940
18	3	4	2	0	3	1	2	1437
19	4	1	2	2	3	0	1	971
20	4	1	3	2	0	3	1	862
21	4	2	1	3	2	0	1	1447
22	4	2	3	0	2	3	1	879
23	4	3	1	3	0	2	1	1564
24	4	3	2	0	3	2	1	1061

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Table 2: Comparison of models with $(m, q) = (4, 3)$.

Model	p	R^2	Adj. R^2
PWO	7	0.9582	0.9435
PWOi	10	0.9717	0.9535
NCP	10	0.9951	0.9919
FOCP	4	0.9571	0.9506
FOCPi	7	0.9705	0.9601
QCP	7	0.9816	0.9751
QCPi	10	0.9951	0.9919
SOCP	12	0.9960	0.9923

(ii) When $3 \leq q < m$, *the full design is D-optimal under the FOCPi model* (3.8) *and the QCPi model* (3.9).

Theorem 3. *When* $3 \leq q < m$, *the full design is D-optimal under the SOCP model* (3.7).

3.3 Summary of Models

We now have presented a series of models for order-of-addition component screening problems with m components and $q < m$ positions. Figure 1 shows the relationship between these models, following Mee (2024). The arrows represent the nested relationship between models, from the smaller one to the larger one. In summary, all component screening models can be categorized into three types: models without component indicators, models

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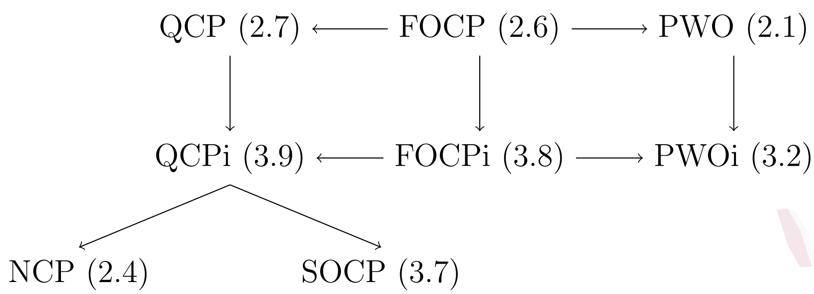

Figure 1: Nesting relationship between order-of-addition models.

with component indicators explicitly, and models with component indicators implicitly, corresponding to the first, second, and third rows in Figure 1, respectively. Models without component indicators do not contain the information of component indicators, and consist of the PWO model (2.1), the FOCP model (2.6) and the QCP model (2.7). Models with component indicators explicitly include the component indicators as additional linear independent variables and consist of the PWOi model (3.2), the FOCPi model (3.8), and the QCPi model (3.9). Finally, models with component indicators implicitly have already contained the information of component indicators in the span of their column spaces, and consist of the NCP model (2.5) and the SOCP model (3.7).

Table 3 gives the numbers of identifiable parameters (p) for all component screening models when $3 \leq q < m$. When $q = 2$, there are not enough positions to entertain quadratic CP effects β_{ii} and therefore the

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Table 3: Model and number of identifiable parameters (p) for $3 \leq q < m$.

Model	Equation	p
PWO	(2.1)	$m(m-1)/2+1$
PWOi	(3.2)	$m(m+1)/2$
NCP	(2.5)	$(m-1)q+1$
FOCP	(2.6)	m
FOCPi	(3.8)	$2m-1$
QCP	(2.7)	$2m-1$
QCPi	(3.9)	$3m-2$
SOCP	(3.7)	$(m+4)(m-1)/2$

QCP, QCPi and SOCP models do not apply. When $q = m$, the component indicators do not provide any information as $S_k(\boldsymbol{x}) = 1$. When $q = 3$, the QCPi and NCP models are equivalent because they have the same number of parameters and the QCPi model is nested within the NCP model.

4. Efficient Component Screening Designs

In the previous section, we have shown that the full design is D-optimal under all component screening models; see Theorems 1–3. However, the full design is often too large and may not be feasible in many practical situations. In this section, we consider the construction of efficient component screening designs with smaller number of runs, and present optimality results under various models.

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4.1 Construction Methods

Stokes and Xu (2024) proposed construction methods for the PWO and NCP models. We briefly recall the three algorithms proposed by Stokes and Xu (2024) as Algorithms 1, 2 and 3. The resulting designs are labelled as $\mathbf{S}_{n,m,q}^{\mathrm{CP}}$ and $\mathbf{S}_{n,m,q}^{\mathrm{PWO}}$, where n is the run size, m is the component size, and $q < m$ is the number of positions available in a run.

Algorithm 1 (Stokes and Xu, 2024)

1: Generate an $n \times m$ design using the first five steps of the algorithm from Stokes and Xu (2022), where m is a prime or prime power.

2: Select the odd-numbered columns first in ascending order, followed by the remaining even-numbered columns, until a total of q columns have been chosen. Permute the q columns to improve its performance under a chosen criterion. Denote the resulting design by $\mathbf{S}_{n,m,q}^{\mathrm{CP}}$.

We first examine the performances of the designs under various models and run sizes with some examples. The run sizes are chosen to fall within the range of each algorithm while maintaining model identifiability. The D-efficiency of a design $\boldsymbol{\xi}$ with model matrix $M(\boldsymbol{\xi})$ is calculated as $D(\boldsymbol{\xi}) = \{|M(\boldsymbol{\xi})|/|M(\boldsymbol{\xi}^*)|\}^{1/p}$, where p is the number of columns of $M(\boldsymbol{\xi})$ and $\boldsymbol{\xi}^*$ is the full design, which is proven to be D-optimal.

Figure 2 presents the D-efficiencies of $\mathbf{S}_{n,m,q}^{\mathrm{CP}}$ constructed from Algo-

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Algorithm 2 (Stokes and Xu, 2024)

1: Generate all tuples (i, j, k) with $1 \le i < j < k \le m$.

2: For every three-component tuple, construct two 3×3 matrices

$$D_{ijk}^{(1)} = \begin{pmatrix} i & k & j \\ j & i & k \\ k & j & i \end{pmatrix} \text{ and } D_{ijk}^{(2)} = \begin{pmatrix} i & j & k \\ j & k & i \\ k & i & j \end{pmatrix}.$$

3: Combine by row-wise concatenating all $D_{ijk}^{(1)}$'s with even $i + j + k$ first and then all $D_{ijk}^{(2)}$'s with odd $i + j + k$.

4: Take the first n rows and denote the resulting design by $\mathbf{S}_{n,m,3}^{\text{PWO}}$.

Algorithm 3 (Stokes and Xu, 2024)

1: For a given smallest optimal q-component OofA-OA, generate the set of $\binom{m}{q}$ q-component OofA-OA's by substituting the levels $(1, 2, \ldots, q)$ with $(i_1, i_2, \ldots, i_q)$, where $1 \le i_1 < i_2 < \cdots < i_q \le m$.

2: Combine the $\binom{m}{q}$ q-component OofA-OA's and arrange the rows systematically such that each of q-component OofA-OAs contributes the same or nearly equal number of rows for the first n rows.

3: Take the first n rows and denote the resulting design by $\mathbf{S}_{n,m,q}^{\text{PWO}}$.

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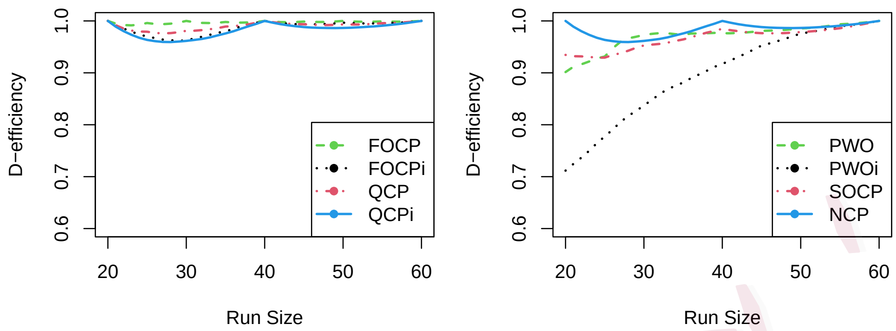

Figure 2: D-efficiencies of $\mathbf{S}_{n,m,q}^{\text{CP}}$ from Algorithm 1 with $(m, q) = (5, 3)$.

rithm 1 with $(m, q) = (5, 3)$ and $n = 20$–60, where columns are permuted to maximize the D-efficiency under the SOCP model by a complete search in Step 2. The SOCP model has the largest number of parameters and maximizing the D-efficiency under the SOCP model tends to yield efficient designs under other models. Overall, the designs perform very well under all models except for the PWOi model, with D-efficiencies of 0.9 or higher. The performances under the PWOi model are the worst, yet the D-efficiencies are still above 0.7. When $n = 60$, this is the full design; as expected, the D-efficiencies reach 1 under all models. When $n = 20$ or 40, the D-efficiencies reach 1 under the FOCP, FOCPi, QCP, QCPi, and NCP models. Since the QCPi and NCP models are equivalent when $q = 3$, we use the solid line for these two models in Figure 2.

Figure 3 presents the D-efficiencies of $\mathbf{S}_{n,m,q}^{\text{PWO}}$ constructed from Algo-

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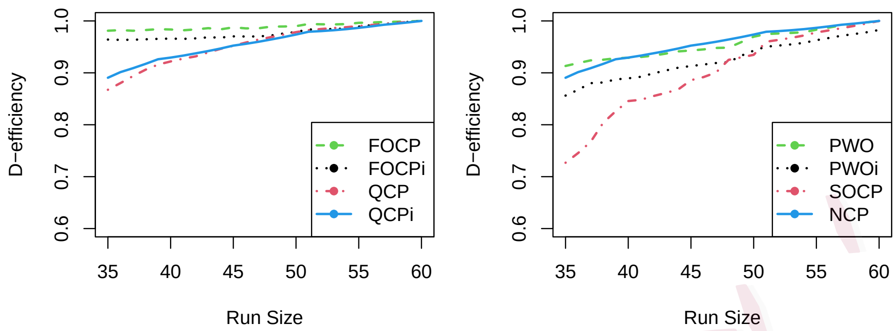

Figure 3: D-efficiencies of $\mathbf{S}_{n,m,q}^{\text{PWO}}$ from Algorithm 2 with $(m, q) = (6, 3)$.

rithm 2 with $(m, q) = (6, 3)$ and $n = 35$–60. The designs perform well under all models. The D-efficiencies are above 0.95 under the FOCP and FOCPi models, above 0.85 under the QCP, QCPi, PWO, PWOi, and NCP models, and above 0.7 under the SOCP model. When $n = 60$, this is a half fraction of the full design, and the D-efficiencies reach 1 under all models except for the PWOi model.

Figure 4 presents the D-efficiencies of $\mathbf{S}_{n,m,q}^{\text{PWO}}$ constructed from Algorithm 3 with $(m, q) = (6, 4)$ and $n = 60$–180. The designs perform well under all models for a wide range of run sizes. The D-efficiencies are above 0.85 under the FOCP, FOCPi, PWO, and PWOi models, and above 0.7 under the QCP, QCPi, NCP, and SOCP models. When $n = 180$, this is a half fraction of the full design, and the D-efficiencies reach 1 under the FOCP, FOCPi, PWO, and PWOi models.

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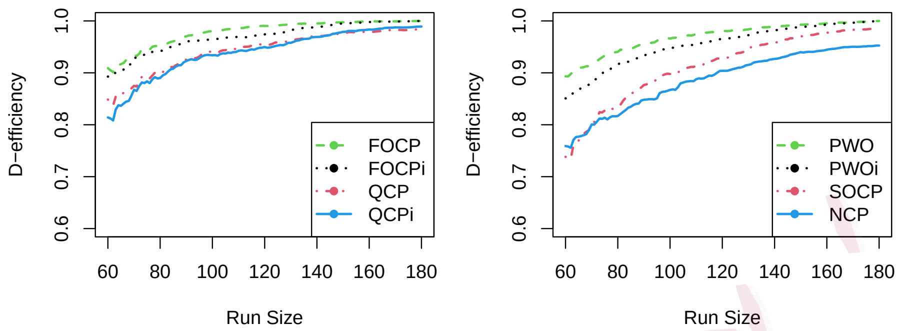

Figure 4: D-efficiencies of $\mathbf{S}_{n,m,q}^{\text{PWO}}$ from Algorithm 3 with $(m, q) = (6, 4)$.

4.2 Design Optimality

To facilitate the description, we extend the concept of a COA to the screening case. An $n \times q$ design is called a COA(n, q, m) if (i) each row is a permutation of q distinct elements from $\{1, 2, \ldots, m\}$ and (ii) for any two columns, all (i, j) combinations for $1 \leq i \neq j \leq m$ appear the same number of times. A COA is also called an orthogonal array of type I by Rao (1961). It is obvious that any q columns of a COA(n, m) form a COA(n, q, m), but not every COA(n, q, m) is a projection of a COA(n, m). For example, a COA$(30, 3, 6)$ exists but COA$(30, 6)$ does not exist (Rao, 1961). We have the following optimality results regarding COAs.

Theorem 4. *If a COA(n, q, m) exists, it is D-optimal under the FOCP, FOCPi, QCP, QCPi, and NCP models.*

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Theorem 4 shows that the condition of being a COA is sufficient for a design to be D-optimal under the FOCP, FOCPi, QCP, QCPi, and NCP models.

The next three theorems summarize the optimality results for the designs constructed from Algorithm 1–3 under various models. For completeness, we include the optimality results from Stokes and Xu (2024), which cover the NCP and PWO models, whereas the results under the other models are new.

Theorem 5. *When n is a multiple of $m(m-1)$, $\boldsymbol{S}^{CP}_{n,m,q}$ constructed from Algorithm 1 is D-optimal under the FOCP, FOCPi, QCP, QCPi, and NCP models.*

By Theorem 1 of Stokes and Xu (2022), when n is a multiple of $m(m-1)$, $\mathbf{S}^{\mathrm{CP}}_{n,m,q}$ constructed from Algorithm 1 is a COA(n, q, m); therefore, Theorem 5 follows from Theorem 4. It confirms the findings in Figure 2 that the D-efficiencies of $\mathbf{S}^{\mathrm{CP}}_{n,m,q}$ from Algorithm 1 reach 1 under the FOCP, FOCPi, QCP, QCPi, and NCP models when the run size n is a multiple of $m(m-1)$, like 20, 40 and 60, for $(m, q) = (5, 3)$.

Theorem 6. *When $n = 3\binom{m}{3}$ and m is even, $\boldsymbol{S}^{PWO}_{n,m,3}$ constructed from Algorithm 2 is D-optimal under the FOCP, FOCPi, QCP, QCPi, NCP and PWO models.*

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Theorem 6 follows from Theorem 5 of Stokes and Xu (2024) and Theorem 4 because $\mathbf{S}^{\mathrm{PWO}}_{n,m,3}$ constructed from Algorithm 2 is a COA$(n,3,m)$ when $n = 3\binom{m}{3}$ and m is even. It confirms the findings in Figure 3 that the D-efficiencies of $\mathbf{S}^{\mathrm{PWO}}_{n,m,3}$ from Algorithm 2 reach 1 under the FOCP, FOCPi, QCP, QCPi, NCP, and PWO models for $(m,q) = (6,3)$ and $n = 60$. On the other hand, $\mathbf{S}^{\mathrm{PWO}}_{n,m,3}$ constructed from Algorithm 2 is not D-optimal under the PWOi model, as $Z_{i,j}(\boldsymbol{x})$ and $S_k(\boldsymbol{x})$ are not orthogonal for distinct i,j,k.

Algorithm 2 and Theorem 6 deal with the special case of $q = 3$. For $q > 3$, Algorithm 3 utilizes the smallest optimal OofA-OA. By Voelkel and Gallagher (2019) and Schoen and Mee (2023), the smallest optimal q-component OofA-OA has $12\lceil(\binom{q}{2}+1)/12\rceil$ runs, where $\lceil x\rceil$ is the smallest integer larger than or equal to x. We have the following result regarding the designs constructed from Algorithm 3.

Theorem 7. *When $3 < q < m$ and $n = 12\lceil(\binom{q}{2}+1)/12\rceil\binom{m}{q}$, $\boldsymbol{S}^{PWO}_{n,m,q}$ constructed from Algorithm 3 is D-optimal under the PWO and PWOi models.*

Theorem 7 confirms the findings in Figure 4 that the D-efficiencies of $\mathbf{S}^{\mathrm{PWO}}_{n,m,q}$ reach 1 under the PWO and PWOi models when the run size is $n = 12\lceil(\binom{q}{2}+1)/12\rceil\binom{m}{q} = 180$ for $(m,q) = (6,4)$. This design does not form a COA(180, 4, 6) because the D-efficiencies are less than 1 under the QCP, QCPi and NCP models.

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5. Simulation Study

Job scheduling problems are a well-known class of NP-hard problems in operations research (Garey et al., 1976). We adopt a single machine model with a quadratic loss function as the true model in our simulation study where one machine is available to process jobs. At each decision point, the machine can be tasked with executing any of the m jobs, with a limit of q jobs to be completed. This problem is common in high-volume manufacturing settings, where processing all jobs is not possible owing to inventory or time constraints (Shabtay et al., 2012, 2013; Zhong et al., 2014). The key parameters encompass the processing time t_i, the waiting cost c_i and the rejection penalty p_i of any unfinished job i for $i = 1, \cdots, m$. Given a scheduling sequence of jobs, denoted as $\boldsymbol{x} = (x_1, \cdots, x_q)$, the corresponding quadratic loss function can be expressed as

$$y(\boldsymbol{x}) = \sum_{i=1}^{q} c_{x_i} (\sum_{j=1}^{i} t_{x_j})^2 + \sum_{k \notin \boldsymbol{x}} p_k. \tag{5.1}$$

We randomly generate 100 sets of time, cost and penalty from the Chi-squared distribution with 2, 2 and 10 degrees of freedom, respectively. We use designs constructed from Algorithm 1, generate the responses according to (5.1), fit various models, and evaluate model fitting and performance. The model performance is evaluated on prediction of the responses at all

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Table 4: Job scheduling parameters.

	Job 1	Job 2	Job 3	Job 4	Job 5	Job 6	Job 7
time	0.30	3.51	3.09	2.48	3.62	1.91	4.25
cost	0.68	0.43	0.23	2.10	0.02	2.05	3.36
penalty	9.82	12.69	5.39	7.36	6.41	9.33	16.22

possible runs in terms of the normalized root mean square error (RMSE), which is defined as

$$\text{Normalized RMSE} = \left[\frac{N^{-1}\sum_{i=1}^{N}\{\hat{y}(\boldsymbol{x}_i) - y(\boldsymbol{x}_i)\}^2}{N^{-1}\sum_{i=1}^{N}\{\bar{y} - y(\boldsymbol{x}_i)\}^2}\right]^{1/2},$$

where N is the run size of the full design, $\boldsymbol{x}_i$ is the ith run of the full design, $y(\boldsymbol{x}_i)$ is the true response (5.1) evaluated at $\boldsymbol{x}_i$, $\hat{y}(\boldsymbol{x}_i)$ is the predicted response from the fitted model, and $\bar{y}$ is the average response of the training data.

We first look into one of the 100 cases with $m = 7$, $q = 4$ and the parameters presented in Table 4. We use a COA$(42, 4, 7)$ constructed from Algorithm 1. Figure 5 presents the component-position effects plot, where each component is represented by a number, the x-axis denotes the position of a component, the y-axis is the mean response conditioning on a certain component and position, and the "NA" position refers to the absence of a component. Looking at positions 1–4, the component-position effects are roughly linear. Among all jobs, job 7 has the largest linear effect over

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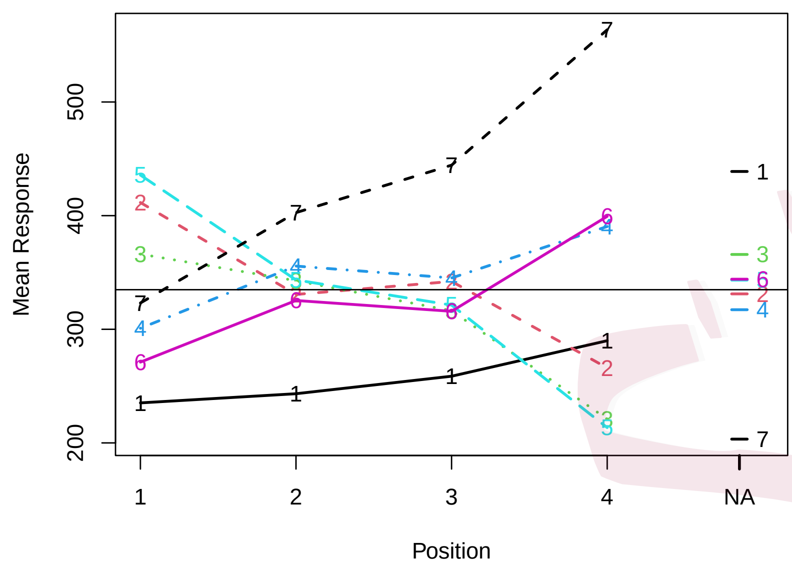

Figure 5: Component-position effects plot for $(m, q) = (7, 4)$ and $n = 42$.

the position (or time) when it is included in a sequence. The earlier it is processed, the smaller the response is. For jobs 5, 2, and 3, the later they are processed, the smaller the responses are. Figure 5 also shows that the difference is large whether jobs 1 and 7 are processed or not. The response is small if job 7 is not included in the sequence whereas the response is large if job 1 is included.

We fit the component screening models to the data. Our investigations focus on the outcomes generated by models with and without component indicators in Table 5. The R^2 values for the five models (FOCPi, QCPi, PWOi, NCP and SOCP) with component indicators are notably higher

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Table 5: Comparison of models with $(m, q) = (7, 4)$.

Model	p	R^2	Adjusted R^2	RMSE
FOCP	7	0.3303	0.2155	0.7933
FOCPi	13	0.9366	0.9103	0.3012
QCP	13	0.3386	0.0649	0.7909
QCPi	19	0.9449	0.9017	0.2947
NCP	25	0.9671	0.9205	0.3256
PWO	22	0.6206	0.2222	1.0594
PWOi	28	0.9828	0.9496	0.2579
SOCP	33	0.9815	0.9159	0.3584

than three models (FOCP, QCP, PWO) without component indicators. The adjusted R^2 values for the FOCP, QCP and PWO models are all below 0.23 whereas that of the other five models are above 0.9. Moreover, the models with component indicators have much smaller RMSE than the three models without component indicators. We conclude that those with component indicators have better goodness of fit and better performance than those without component indicators. The FOCPi and QCP models have the same number of parameters, but the FOCPi model has much higher R^2 and adjusted R^2 values than the QCP model, further validating that component indicators matter. The PWOi model has the largest R^2 and adjusted R^2 values, and the smallest RMSE value. The FOCPi model performs very well even though it has the smallest number of parameters among the models

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with component indicators. It outperforms the NCP and SOCP models in terms of model prediction.

Afterwards, we systematically examine 100 randomly generated true parameter settings to assess the consistency of specific patterns across different cases. Figure 6 shows the comparison of model performances in terms of R^2 and normalized RMSE. It is evident that the inclusion or exclusion of component indicators produces substantial differences in both measures. The five models with component indicators fit the data much better and has much smaller RMSE than the three models without component indicators. The five models with component indicators are quite competitive. Remarkably, these patterns also persist across varying pairs of (m, q), which is not shown here.

In addition, we extend our investigation to utilize designs constructed from Algorithms 1, 2 and 3. The results are similar so they are omitted. In conclusion, the proposed models are useful in capturing the variability of job scheduling mechanism.

6. Concluding Remarks

We propose a series of novel models designed to address scenarios where both the component order and the component selection play crucial roles

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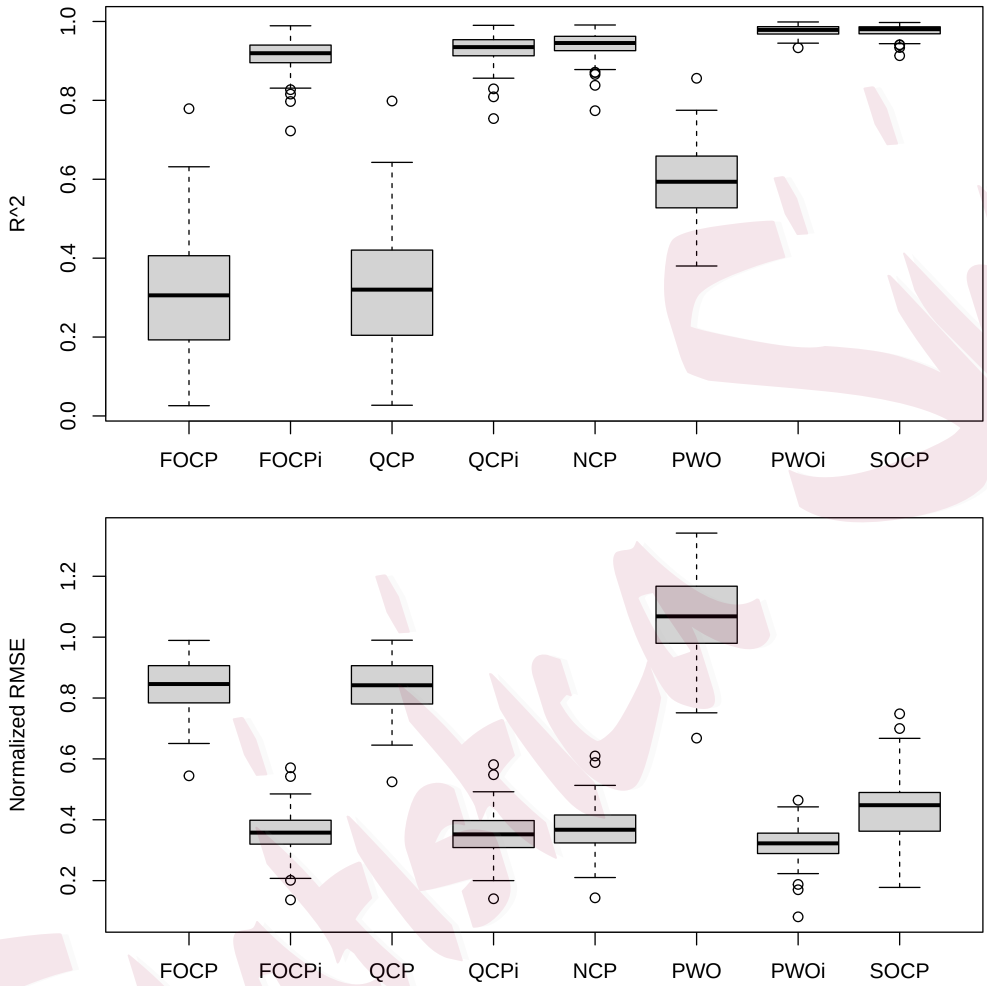

Figure 6: Comparison of models with $(m, q) = (7, 4)$ and $n = 42$ in terms of R^2 (top) and RMSE (bottom).

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in the model effects. Our models combine the order-of-addition effects proposed by Stokes and Xu (2024) with component indicators. We also extend the quantitative CP models proposed by Stokes and Xu (2022) to screening experiments. Based on the effects considered above, we discuss the properties and relationship between these models. We prove that the full design is D-optimal across all models. We further consider smaller designs and establish the D-optimality under their respective models except for the SOCP model. COAs (of strength two) are no longer D-optimal for the SOCP model because it includes the interactions. It would be interesting to construct D-optimal or D-efficient fractional designs under the SOCP model, possibly by searching for COAs of strength three or more.

Through examples and simulations, we demonstrate that the newly proposed models are useful in addressing the job scheduling and component screening problems. It is not uncommon that several models may fit the same data equally well. When analyzing real-world data, a data-driven testing procedure may be necessary to determine a final model formally. One may use any standard procedure such as stepwise regression with the AIC or BIC criterion.

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Supplementary Material

The online Supplementary Material contains the proofs.

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