Integer Programming Approaches to Find Row-Column Arrangements of Two-Level Orthogonal Experimental Designs

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Abstract

Design of experiments is an effective, generic methodology for problem solving as well as for improving or optimizing product design and manufacturing processes. The most commonly used experimental designs are two-level fractional factorial designs. In recent years, nonregular fractional factorial two-level experimental designs have gained much popularity compared to the traditional regular fractional factorial designs, because they offer more flexibility in terms of run size as well as the possibility to estimate partially aliased effects. For this reason, there is much interest in finding good nonregular designs, and in orthogonal blocking arrangements of these designs. In this contribution, we address the problem of finding orthogonal blocking arrangements of high-quality nonregular two-level designs in scenarios with two crossed blocking factors. We call these blocking arrangements orthogonal row-column arrangements. We propose two strategies to find row-column arrangements of given two-level orthogonal treatment designs such that the treatment factors' main effects are orthogonal to both blocking factors. The first strategy involves a sequential approach which is especially useful when one blocking factor is more important than the other. The second strategy involves a simultaneous approach for situations where both blocking factors are equally important. For the latter approach, we propose three different optimization models, so that, in total, we consider four different methods to obtain row-column arrangements. We compare the performance of the four methods by looking for good row-column arrangements of the best two-level 24-run designs in terms of the G-aberration criterion, and apply the best of these methods to 64- and 72-run orthogonal designs.

KEY WORDS: Aliasing; Confounding; Generalized Word-Length Pattern; Integer Linear Programming; Crossed Blocking Factors; Row-Column Design.

1 Introduction

1.1 Experimental design

Experimental designs play an important role in industrial engineering, as they are key tools in the context of product and process innovation or improvement. More specifically, experimental designs define a plan for a systematic study of the relationship between one or more outputs of a process and controllable inputs to that process, or between one or more measures of a product's performance and characteristics of that product. Generally, we use the name factor or treatment factor for each process input or for each product characteristic studied in an experiment. In the initial phase of a study, experiments typically involve a large number of factors and two levels are used for each factor. A full factorial experimental design involves

all possible combinations of the two levels of the factors. Usually, this experimental design is much too large to be practically feasible. Fractional factorial experimental designs involve only a fraction of the test combinations of the full factorial design. Depending on the cost of the experimental tests and the time available for the entire experiment, a small fraction or a larger fraction of the test combinations in the full factorial design will be chosen. Experiments in which the number of factors studied is large compared to the number of tests performed (also called number of runs) are often referred to as screening experiments.

For many years, the two-level fractional factorial experimental designs used for screening experiments were regular. The main advantage of regular fractional factorial designs is that they can be constructed by hand using so-called design generators, which are tabulated in textbooks such as Wu and Hamada (2009) and Mee (2009) and which are available in design of experiments software. One main drawback of regular fractional factorial designs is that they offer little flexibility in terms of the size of the experiment: the number of experimental tests (which, in the jargon, is called the run size) should be a power of 2. Another drawback is that regular fractional factorial designs generally involve effects that are completely aliased with each other, as a result of which certain effects of the factors cannot be disentangled. In recent years, much research has been spent on nonregular two-level fractional factorial designs, because these designs exist for any number of tests that is a multiple of 4 and because many nonregular fractional factorial designs do not involve completely aliased factor effects (Mee, 2009; Schoen and Mee, 2012; Schoen et al., 2017).

1.2 Need for blocking

Ideally, experimental designs should be completely randomized and all tests should be conducted under homogeneous circumstances. So, the environment in which the experiment is carried out should be controlled to the maximum possible extent, to ensure that the experimental tests are not impacted by sources of variation other than the experimental factors. Many experiments, however, span multiple days, require multiple batches of raw material and involve multiple climate chambers, operators or machines. For the experimental design to be as informative as possible and for a suitable data analysis, it is important to account for any heterogeneity due to days, batches, climate chambers, operators or machines, for instance. This principle is referred to as blocking in the experimental design literature (Wu and Hamada, 2009; Goos and Jones, 2011).

The factors that define the heterogeneous conditions are called blocking factors. In the presence of one or more blocking factors, the experimental runs are grouped, each group is called a block and corresponds to a different level of a blocking factor. The goal of blocking is to ensure no unwarranted conclusions are drawn from the data analysis and that the quantification or estimation of the factors' effects is impacted as little as possible by the heterogeneity of the experimental conditions. To this end, the experiment should be designed in such a way that the effects of the treatment factors are confounded with the blocks to the smallest possible extent.

Blocking plays an important role in experiments in industry, agriculture, food technology, bioprocessing and pharmaceutics. For example, the glasshouse experiment in Williams and John (1996) involves six replicates of a design with two treatment factors along with a four-level and an eight-level blocking factor. The treatment factors were salt-irrigation level and seed lot. The two blocking factors were related to the physical arrangement of the experimental tests in the glasshouse: it was known from previous experiments in the glasshouse that conditions affecting growth varied considerably both down the north-south length of the glasshouse and also from the sides to the center. The first blocking factor thus is the position along the north-south length, while the second blocking factor is the position along the east-west axis. Another example of an experiment involving two blocking factors is the pastry dough experiment described by Gilmour and Trinca (2003), which required seven days, and, within a day, the runs were performed at four different times. Therefore, the pastry dough experiment also involved two blocking factors. Finally, Goos and Donev (2006a,b) mention a valve wear experiment, where the two blocking factors are the valve position and the engine, and a food additives experiment, where the two blocking factors are the enzyme supplier and the batch of wheat.

A key feature of the two blocking factors in each of these examples is that they are crossed. This is because every level of one blocking factor is used at each level of the other blocking factor, and vice versa. For instance, in the pastry dough experiment, each of the four time points is used on each day, and, at each time point, one test is performed on each of the seven days. Typically, experimental designs with two crossed

Table 1: A four-factor two-level treatment design with 24 runs arranged in four rows and three columns, with two runs for each combination.

	Batch 1				Batch 2				Batch 3			
Day 1	−1	1	1	−1	−1	1	1	1	−1	1	1	1
	1	−1	−1	−1	1	−1	−1	1	1	−1	−1	−1
Day 2	−1	−1	1	1	−1	−1	1	−1	−1	−1	1	−1
	1	1	−1	−1	1	1	−1	1	1	1	−1	1
Day 3	−1	1	−1	1	−1	1	−1	−1	−1	1	−1	−1
	1	−1	1	−1	1	−1	1	1	1	−1	1	1
Day 4	−1	−1	−1	1	−1	−1	−1	−1	−1	−1	−1	1
	1	1	1	1	1	1	1	−1	1	1	1	−1

blocking factors are called row-column designs, where the rows and the columns represent the levels of the first blocking factor and the levels of the second blocking factor, respectively.

This paper focuses on row-column designs for two-level fractional factorial experiments. As an example, suppose that an experimenter wants to investigate the effect of the treatment factors seeding density, medium, the addition of serum to the medium and exposure time on the viability of cells exposed to a surface pollutant. For each of the factors, two levels are selected, and these are coded with -1 and 1. The budget allows for 24 tests or, in the experimental design jargon, runs. However, the cells used in the experiment originate from several batches which may be slightly different. One batch supplies cells for eight runs only. So, three batches are needed to cover the intended 24 runs. In addition, the experimenters can handle six runs per day. As a result, four days are needed to handle all 24 runs. In conclusion, the 24 runs should be arranged in four rows, corresponding to the days, and three columns, corresponding to the batches.

In Table 1, we show a suitable experimental design for the viability example. There are 12 combinations of day and batch. For each of these combinations, there are two runs. Each run involves a particular combination of the levels of the four treatment factors. These combinations are shown as tuples with four elements.

After carrying out the experiment and observing the viability of the cells in the 24 experimental runs, a statistical model needs to be built to relate the viability to the levels of the treatment factors. That model should also account for the variability caused by the different batches and days. Generally, the following model is considered:

$$Y_{ijk} = \beta_0 + \sum_{l=1}^{4} \beta_l x_{ijkl} + \sum_{l=1}^{3} \sum_{m=l+1}^{4} \beta_{lm} x_{ijkl} x_{ijkm} + \gamma_i + \delta_j + \varepsilon_{ijk}, \tag{1}$$

where Y_{ijk} represents the viability observed at the kth test on day i using batch j and $x_{ijk1}, \ldots, x_{ijk4}$ represents the levels of the four treatment factors at that test. Generally, Y_{ijk} is referred to as the response. The parameters β_0, $\beta_1, \ldots, \beta_4$ and $\beta_{12}, \ldots, \beta_{34}$ represent the intercept, the treatment factors' main effects and their second-order or two-factor interaction effects, respectively. The parameters γ_i and δ_j represents the effects of the ith day and the jth batch on the response. Finally, ε_{ijk} is the random error at the kth test on day i using batch j. The parameters of the statistical model are generally estimated using the least squares method (Wu and Hamada, 2009). This approach treats the row and column effects γ_i and δ_j as unknown fixed parameters, just like the other model parameters (Goos and Jones, 2011).

The two-factor interaction effects are relevant whenever the effect of one factor on the response depends on the level of another factor. A major advantage of factorial experimental designs is that two-factor interaction effects can be quantified. However, main effects generally explain a larger proportion of the variation in the response than interaction effects (Wu and Hamada, 2009). It is therefore preferably to prioritize the estimation of the main effects. Because orthogonal two-level experimental treatment designs guarantee a precise, independent estimation of the main effects, many experimenters exclusively utilize such

designs. Whenever the experiment is complicated by the presence of blocking factors, it is desirable that the experimental treatment design is orthogonally blocked. This is achieved by making sure that the levels of the treatment factors are orthogonal to each of the blocking factors. Orthogonal blocking preserves the precise, independent estimation of the main effects. Ideally, also the interaction effects can be estimated precisely and independently, both in the absence and presence of blocking factors. However, in order to obtain precise, independent estimates of the interactions, large experiments are required. The experimental design in Table 1 is an orthogonal treatment design that is orthogonally blocked with respect to the days and the batches. So, it is an orthogonal row-column design.

1.3 Goal and outline of this paper

A major conclusion from our literature review in Section 2 is that it is unknown how to optimally arrange the runs of attractive nonregular two-level fractional factorial treatment designs with 32 runs or more in rows and columns to create orthogonal row-column designs. In the present paper, we address this problem by taking a given orthogonal treatment design with good statistical features and arranging it in a rows and b columns such that the complete row-column design is also an orthogonal design. In other words, we ensure that the treatment design is orthogonally blocked with respect to the rows and with respect to the columns. To this end, we extend the approach of Sartono et al. (2015, SSG), who propose a mixed integer linear programming approach to create an orthogonal blocking arrangement for a two-level nonregular treatment design in the event there is a single blocking factor. More specifically, we extend their method to deal with two crossed blocking factors. We show that this extension can be done in several ways, and we compare the resulting blocking arrangements and the computing times for each approach. The ultimate goal of our work is to find row-column arrangements which allow the independent estimation of all main effects of the treatment factors and block effects, and the estimation of as many two-factor interaction effects as possible.

Throughout this article, we assume that a high-quality two-level orthogonal treatment design is used as the starting point for creating a row-column design. By a high-quality design, we mean a minimum G- or G_2-aberration strength-2 orthogonal design or a strength-3 orthogonal design. In the literature, much research has already been done concerning such designs, so that high-quality two-level orthogonal treatment designs are readily available. We refer to Block and Mee (2005), Xu and Wong (2007), Cheng et al. (2008), Mee (2009), Xu (2009), Schoen and Mee (2012), Eendebak and Schoen (2017) and Schoen et al. (2017) for recent studies on two-level orthogonal treatment designs.

The remainder of this paper is organized as follows. Section 2 contains a literature review. In Section 3, we introduce the notation and the main concepts we used. Next, in Section 4.1, we embed the mixed integer linear programming approach of SSG in a two-stage procedure that arranges two-level treatment designs in rows first, and then in columns. We refer to this two-stage procedure as the sequential approach. In Section 4.2, we propose three different optimization models to arrange the two-level designs in rows and columns simultaneously. In Section 5, we apply the four approaches to construct 24-run row-column designs, compare the designs found with those from the literature, and study the computing times. This allows us to select the most appropriate approaches to search for row-column arrangements of 64- and 72-run treatment designs. A discussion in Section 6 concludes the paper.

2 Literature review

Row-column designs for factorial experiments have been studied extensively. Jacroux and SahaRay (1990), for example, proposed a design construction method for two-level treatment designs. They arranged either a full factorial design or a regular fractional factorial design involving $m + n$ factors in 2^m rows and 2^n columns so that the resulting designs can be used to estimate all main effects independently of the block effects. Their approach has two major limitations. First, the number of runs and the number of rows and columns must be powers of 2. Second, their approach cannot deal with experiments involving more than one run at each row-column combination (such as the viability experiment discussed in the introduction of this paper). Williams and John (1996) proposed a computer algorithm to construct row-column arrangements of factorial designs which allow a precise estimation of main effects, while ignoring the interaction effects.

Based on weighted mean efficiency factors, Gilmour and Trinca (2003) proposed an algorithm for creating factorial row-column designs for quantitative factors and a response surface model. Their construction

involves an interchange algorithm (Jones and Eccleston, 1980), and treats the block effects (i.e., the row and column effects) as fixed. Goos and Donev (2006a,b) proposed a point-exchange algorithm to construct D-optimal row-column designs when the block effects are either treated as random or as fixed. The approaches of Gilmour and Trinca (2003) and Goos and Donev (2006a,b) require the number of experimental runs to be large enough to estimate the model involving all main effects and all two-factor interaction effects. In this paper, we focus on screening experiments which, generally, do not allow all two-factor interaction effects to be estimated at the same time. This is because, in screening experiments, the number of runs is generally small relative to the total number of effects in a main-effects-plus-interactions model.

Based on the estimation capacity criterion, Cheng and Mukerjee (2003) provided a methodology to construct s^{n-k} fractional factorial designs, involving s levels for each of n treatment factors, in s^r rows and s^c columns. Their approach has two major limitations. First, the number of runs and the number of rows and columns must be powers of s. Second, because they use regular designs, the resulting row-column designs involve completely aliased effects.

In order to overcome these limitations, Vo-Thanh et al. (2019) proposed a general method to search for nonregular row-column designs with two-level treatment factors, starting from complete catalogs of non-isomorphic orthogonal arrays of the type $\text{OA}(N, a \times b \times 2^n, t)$, where N, a, b, n, and t represent the run size, the number of levels of the first blocking factor (corresponding to the rows of the row-column design), the number of levels of the second blocking factor (corresponding to the columns of the row-column design), the number of two-level treatment factors, and the strength of the design. An orthogonal array is of strength t if, for any given subset of t factors, all combinations of levels occur equally often. The orthogonal arrays used most frequently have a strength of 2 or 3. Orthogonal arrays of strength 2 offer the advantage that the main effects can be estimated independently and with maximum precision, in the event no interaction effects are present. Orthogonal arrays of strength 3 offer the same advantages even in the presence of interactions.

Unfortunately, for run sizes larger than or equal to 32, it is computationally infeasible to generate and explore complete catalogs of non-isomorphic orthogonal arrays of the type $\text{OA}(N, a \times b \times 2^n, 2)$. Therefore, searching for optimal row-column arrangements of orthogonal arrays of the type $\text{OA}(N, 2^n, 2)$ using the methods of Vo-Thanh et al. (2019) is not feasible for $N \geq 32$. For larger run sizes, Vo-Thanh et al. (2019) instead explore catalogs of strength-3 orthogonal arrays of the type $\text{OA}(N, a \times b \times 2^n, 3)$. However, the usefulness of this approach is limited because it requires both the full row-column design and the two-level treatment design to be of strength 3. This requirement is too strict because experimenters generally assume that there are no interactions between the blocking factors and the treatment factors (Wu and Hamada, 2009). Therefore, it is sufficient for the full row-column design to have a strength of 2, while the treatment design has a strength of 3.

Even for one single strength-3 treatment design, the number of different extensions to a row-column design of the type $\text{OA}(N, a \times b \times 2^n, 2)$ can be too big to enumerate completely for $N \geq 32$. Consequently, it is unknown how to optimally arrange, for example, the runs of the large number of attractive two-level treatment designs of strength 3 identified by Schoen and Mee (2012) in rows and columns to create row-column designs. What is needed is methodology that is able to arrange any strength-3 treatment design in a rows and b columns such that the entire row-column design, including the treatment factors and the two blocking factors, is of the type $\text{OA}(N, a \times b \times 2^n, 2)$.

3 Preliminaries

In this section, we introduce the concepts relevant for the optimization models that we developed to arrange regular or nonregular two-level treatment designs in rows and columns, and we illustrate them by revisiting the viability experiment in Section 1.2. Following the literature on blocked experiments (Bailey, 2008; Wu and Hamada, 2009; Vo-Thanh et al., 2019), we assume that there are no interactions between the first blocking factor (corresponding to the rows) and the second blocking factor (corresponding to the columns), and that there are no interactions between the blocking factors and the treatment factors. Also, since experimenters using two-level screening designs are generally only interested in main effects and two-factor interaction effects, we restrict our attention to these effects. This implies that our construction of row-column designs assumes that the statistical model in Equation (1) will be used for analyzing the resulting data. In many cases, however, the experiment is not large enough to estimate all parameters β_0, $\beta_1, \ldots, \beta_4$ and $\beta_{12}, \ldots, \beta_{34}$ in the statistical model simultaneously. As our approach does not require all parameters to

be estimable simultaneously, this is not problematic.

3.1 Quality measures for two-level treatment designs

The two-level treatment designs considered in this paper are derived from orthogonal arrays. There may be many treatment designs with N runs, n treatment factors and strength t. Designs that can be obtained from each other by row permutations, column permutations and level permutations in the columns are statistically equivalent and belong to the same isomorphism class. We denote a catalog of orthogonal arrays in which a single representative of every isomorphism class is included by $\mathrm{OA}(N, 2^n, t)$, and we call this set the set of non-isomorphic designs with parameters N, n and t. Also, we denote the two levels of each treatment factor by -1 and 1.

For the viability experiment mentioned in Section 1, 24 runs were feasible to investigate four treatment factors. So, $N = 24$ and $n = 4$ for that example. It turns out that there exist two statistically different strength-3 orthogonal arrays for these values of N and n. In other words, there are two non-isomorphic designs in $\mathrm{OA}(24, 2^4, 3)$ (Schoen et al., 2010). One of these designs is shown in Table 1 in a row-column arrangement. An alternative representation of that design is shown in the first four columns of Table 2. The design is denoted by the matrix $\mathbf{X}$, which in this case has 24 rows and four columns. In general, $\mathbf{X}$ is an $N \times n$ matrix with N runs and n factors. Every column of $\mathbf{X}$ is called a main-effect contrast column. In the table, the four main-effect contrast columns are labeled with **1**, **2**, **3** and **4**, respectively. The elements of the main-effect contrasts columns correspond to the values $x_{ijk1}, \ldots, x_{ijk4}$ in the statistical model in Equation (1).

Every treatment design matrix $\mathbf{X}$ has a corresponding $(N \times q)$-dimensional two-factor interaction contrast matrix $\mathbf{W}$, where $q = n(n-1)/2$ represents the number of two-factor interaction effects. The matrix $\mathbf{W}$ is obtained by element-wise multiplication of all pairs of main-effect contrast vectors in $\mathbf{X}$. We denote the element in the ith row and jth column of $\mathbf{W}$ by w_{ij}. In Table 2, the matrix $\mathbf{W}$ for the viability example is shown next to the treatment design $\mathbf{X}$. It has six columns, which are denoted by combining the labels of two main-effect contrast columns. Another way of putting this is to say that the matrix $\mathbf{W}$ contains the values of the cross-products $x_{ijkl}x_{ijkm}$ from the model in Equation (1).

The treatment design shown in Tables 1 and 2 is one of the two possible options in $\mathrm{OA}(24, 2^4, 3)$. Ideally, we select the best of these two options as input to our methodology for arranging treatment designs in rows and columns. One of the best-known criteria for selecting a good two-level design option is the G-aberration criterion originally proposed by Deng and Tang (1999). Using this criterion requires calculating the so-called J_k-characteristics of k-factor interaction contrast vectors. These are calculated by taking the element-wise product of the k factors, summing the entries and taking the absolute value of the result. For experimental designs consisting of orthogonal arrays, all J_1- and J_2-characteristics equal zero. A J_3-characteristic quantifies the correlation between main-effect contrast vectors and two-factor interaction contrast vectors, while a J_4-characteristic quantifies the correlation among two-factor interaction contrast vectors. The G-aberration criterion is based on the frequencies with which the various J_k-characteristic values occur across all subsets of k factors. These frequencies are collected in frequency vectors. There is one frequency vector for each value of $k \geq 3$. The minimum G-aberration treatment design is the one that sequentially minimizes the entries of the frequency vectors, starting with the entries of the frequency vector for $k = 3$, followed by the entries of the frequency vector for $k = 4$, etc. This way, the least desirable kinds of aliasing are avoided as much as possible. This ensures that the main effects β_l and the interaction effects β_{lm} can be estimated as well as possible.

The two non-isomorphic candidate designs for the viability experiment have a strength of 3. Therefore, the main-effect contrast vectors are uncorrelated with the two-factor interaction contrast vectors and all J_3-characteristics equal zero. There is a single J_4-characteristic for each of the candidate designs, because there is just one set of four vectors to calculate such a characteristic. Its value equals 8 for the design option shown in Table 2 and 24 for the other option. All strength-2 designs, collected in the catalog labeled $\mathrm{OA}(24, 2^4, 2)$, have at least one J_3-characteristic larger than zero. Therefore, the treatment design shown in Tables 1 and 2 is the minimum G-aberration design.

Tang and Deng (1999) proposed an alternative to the G-aberration criterion which they called the G_2-aberration criterion. This criterion ranks designs based on the generalized word length pattern, $W = (A_1, A_2, \ldots, A_n)$. For treatment designs based on orthogonal arrays, $A_1 = A_2 = 0$. The entry A_3 quantifies

Table 2: Alternative representation of the treatment design in Table 1, along with the suboptimal row-column arrangement shown in that table and with the optimal row-column arrangement. The first four columns show the main-effect contrast vectors $x_{ijk1}, \ldots, x_{ijk4}$ in $\mathbf{X}$, while the next six show the two-factor interaction contrast vectors $x_{ijk1}x_{ijk2}, \ldots, x_{ijk3}x_{ijk4}$ in $\mathbf{W}$. The suboptimal and the optimal row-column arrangements are indicated using the assignment matrices $\mathbf{A}$ and $\mathbf{B}$.

X				**W**						Suboptimal		Optimal	
1	**2**	**3**	**4**	**12**	**13**	**14**	**23**	**24**	**34**	**A**	**B**	**A**	**B**
−1	−1	−1	−1	1	1	1	1	1	1	0 0 0 1	0 1 0	1 0 0 0	1 0 0
−1	−1	−1	1	1	1	−1	1	−1	−1	0 0 0 1	1 0 0	0 1 0 0	0 0 1
−1	−1	−1	1	1	1	−1	1	−1	−1	0 0 0 1	0 0 1	0 0 0 1	0 1 0
−1	−1	1	−1	1	−1	1	−1	1	−1	0 1 0 0	0 1 0	0 0 1 0	0 0 1
−1	−1	1	−1	1	−1	1	−1	1	−1	0 1 0 0	0 0 1	0 0 0 1	0 1 0
−1	−1	1	1	1	−1	−1	−1	−1	1	0 1 0 0	1 0 0	0 1 0 0	1 0 0
−1	1	−1	−1	−1	1	1	−1	−1	1	0 0 1 0	0 1 0	1 0 0 0	0 0 1
−1	1	−1	−1	−1	1	1	−1	−1	1	0 0 1 0	0 0 1	0 1 0 0	0 1 0
−1	1	−1	1	−1	1	−1	−1	1	−1	0 0 1 0	1 0 0	0 0 1 0	1 0 0
−1	1	1	−1	−1	−1	1	1	−1	−1	1 0 0 0	1 0 0	0 0 1 0	1 0 0
−1	1	1	1	−1	−1	−1	1	1	1	1 0 0 0	0 1 0	1 0 0 0	0 1 0
−1	1	1	1	−1	−1	−1	1	1	1	1 0 0 0	0 0 1	0 0 0 1	0 0 1
1	−1	−1	−1	−1	−1	−1	1	1	1	1 0 0 0	1 0 0	0 0 1 0	0 1 0
1	−1	−1	−1	−1	−1	−1	1	1	1	1 0 0 0	0 0 1	0 0 0 1	0 0 1
1	−1	−1	1	−1	−1	1	1	−1	−1	1 0 0 0	0 1 0	1 0 0 0	1 0 0
1	−1	1	−1	−1	1	−1	−1	1	−1	0 0 1 0	1 0 0	0 1 0 0	1 0 0
1	−1	1	1	−1	1	1	−1	−1	1	0 0 1 0	0 1 0	1 0 0 0	0 0 1
1	−1	1	1	−1	1	1	−1	−1	1	0 0 1 0	0 0 1	0 0 1 0	0 1 0
1	1	−1	−1	1	−1	−1	−1	−1	1	0 1 0 0	1 0 0	0 0 0 1	1 0 0
1	1	−1	1	1	−1	1	−1	1	−1	0 1 0 0	0 1 0	0 1 0 0	0 1 0
1	1	−1	1	1	−1	1	−1	1	−1	0 1 0 0	0 0 1	0 0 1 0	0 0 1
1	1	1	−1	1	1	−1	1	−1	−1	0 0 0 1	0 1 0	1 0 0 0	0 1 0
1	1	1	−1	1	1	−1	1	−1	−1	0 0 0 1	0 0 1	0 1 0 0	0 0 1
1	1	1	1	1	1	1	1	1	1	0 0 0 1	1 0 0	0 0 0 1	1 0 0

the extent to which main effects are aliased with two-factor interactions, the entry A_4 quantifies the extent to which two-factor interactions are aliased with other two-factor interactions, etc. A minimum G_2-aberration design sequentially minimizes the generalized word length pattern, starting with the A_3 value, followed by the A_4 value, etc. As experimenters' interest is usually only in main effects and two-factor interaction effects, it is common to consider only the A_3 and A_4 values when selecting an appropriate treatment design.

The treatment design shown in Tables 1 and 2 has $A_3 = 0$ and $A_4 = 1/9$. The alternative strength-3 design has $A_3 = 0$ and $A_4 = 1$. All strength-2 designs in $\mathrm{OA}(24, 2^4, 2)$ have $A_3 > 0$. For this reason, the treatment design in Tables 1 and 2 is a minimum G_2-aberration design as well as as a minimum G-aberration design.

3.2 Quality measures for row-column arrangements

Our primary goal is to arrange any given treatment design $\mathbf{X}$ in rows and columns so that we can estimate a model containing all main effects β_l, the block effects γ_i and δ_j (corresponding to the rows and the columns), and as many two-factor interaction effects β_{lm} as possible. In addition, we desire the main-effect estimates to be independent from the block effects. To achieve these goals, (i) the main-effect contrast vector in $\mathbf{X}$ have to be orthogonal to the blocks effects (i.e., the row and the column effects), (ii) the row and the column blocking factors have to be orthogonal to each other, and (iii) the two-factor interaction contrast vectors have to be as orthogonal as possible to the block effects. It is common to say that the main effects should not be confounded with the block effects (which rephrases condition (i)), and that the two-factor interactions should be confounded with the blocks as little as possible (which rephrases condition (iii)).

We denote the number of levels of the row factor (i.e., the first blocking factor) by a, and the number of levels of the column factor (i.e., the second blocking factor) by b. The assignment of the treatments to the rows is represented by the $(N \times a)$-dimensional binary matrix $\mathbf{A}$. An element a_{ij} of $\mathbf{A}$ takes the value 1 when the ith run of the treatment design $\mathbf{X}$ is assigned to the jth row, and 0 otherwise. The assignment of the treatments to the columns is represented by the $(N \times b)$-dimensional matrix $\mathbf{B}$. An element b_{ij} of $\mathbf{B}$ takes the value 1 when the ith run of $\mathbf{X}$ is assigned to the jth column, and 0 otherwise. A necessary condition for an orthogonal row-column arrangement to exist is that N/a and N/b should be even.

The $\mathbf{A}$ and $\mathbf{B}$ matrices corresponding to the row-column arrangement in Table 1 are shown in Table 2 under the heading 'Suboptimal'. The $\mathbf{A}$ and $\mathbf{B}$ matrices corresponding to the best possible arrangement in rows and columns are shown under the heading 'Optimal'. To illustrate the correspondence between the suboptimal $\mathbf{A}$ and $\mathbf{B}$ matrices and the arrangement in Table 1, we focus on the first run in the design. At this run, all treatment factors act at their -1 level. The first three elements in the first row of the $\mathbf{A}$ matrix are zero, while the fourth element is 1. This indicates that the first run is allocated to the fourth row of the row-column arrangement (corresponding to day 4). Similarly, the fact that the second element of the first row of the $\mathbf{B}$ matrix equals 1 indicates that the run is allocated to the second column of the row-column arrangement (corresponding to batch 2). It is easy to verify in Table 1 that the run whose factor levels are all -1 is indeed allocated to day 4 and batch 2.

When ignoring the interaction effects, and thus considering only the main effects of the four treatment factors in Tables 1 and 2, the suboptimal and optimal row-column arrangements in Table 2 are equally good. This is because the four treatment factors are orthogonal to the rows and the columns for both row-column arrangements. As a matter of fact, the levels of each individual factor sum to zero within any row as well as within any column. However, when considering the confounding of the two-factor interactions with the rows and columns, the two row-column arrangements in Table 2 are no longer equivalent.

We quantify the confounding of the two-factor interaction effects with the rows using the $(q \times a)$-dimensional matrix $\mathbf{S}_A = \mathbf{W}^T\mathbf{A}$ and the confounding of the two-factor interaction effects with the columns using the $(q \times b)$-dimensional matrix $\mathbf{S}_B = \mathbf{W}^T\mathbf{B}$. We denote the elements of $\mathbf{S}_A$ and $\mathbf{S}_B$ by s_{ij}^A and s_{ij}^B, respectively. An element s_{ij}^A measures the extent to which the ith two-factor interaction is confounded with the jth level of the first blocking factor (i.e., with the jth row of the row-column arrangement). An element s_{ij}^B measures the extent to which the ith two-factor interaction is confounded with the jth level of the second blocking factor (i.e., with the jth column of the row-column arrangement). Ideally, all s_{ij}^A and s_{ij}^B values are zero, in which case there is no confounding of the treatments factors' second-order interactions with the blocks and the two-factor interaction contrast vectors in $\mathbf{W}$ are orthogonal to the rows and to the columns. The more positive or negative the s_{ij}^A and s_{ij}^B values, the more substantial is the confounding with the blocks

Table 3: $\mathbf{S}_A$ and $\mathbf{S}_B$ matrices quantifying the confounding between the two-factor interaction contrast vectors in $\mathbf{W}$ in Table 2, on the one hand, and the rows and columns, on the other hand. The symbols r_i and c_j refer to the four rows and the three columns of the row-column arrangement.

Contrast	Suboptimal $\mathbf{S}_A$				Suboptimal $\mathbf{S}_B$			Optimal $\mathbf{S}_A$				Optimal $\mathbf{S}_B$		
	r_1	r_2	r_3	r_4	c_1	c_2	c_3	r_1	r_2	r_3	r_4	c_1	c_2	c_3
12	−6	6	−6	6	0	0	0	−2	2	−2	2	0	0	0
13	−6	−6	6	6	0	0	0	2	2	−2	−2	0	0	0
14	−2	2	2	−2	−4	4	0	2	−2	2	−2	0	0	0
23	6	−6	−6	6	0	0	0	2	−2	−2	2	0	0	0
24	2	2	−2	−2	0	0	0	−2	−2	2	2	0	0	0
34	2	−2	2	−2	0	0	0	2	−2	−2	2	0	0	0

(i.e., the rows and the columns). Finally, we denote the maximum absolute elements of the matrices $\mathbf{S}_A$ and $\mathbf{S}_B$ by s_A and s_B, respectively.

The $\mathbf{S}_A$ and $\mathbf{S}_B$ matrices for the suboptimal and optimal row-column arrangements for the minimum G- and G_2-aberration design for the viability experiment in Table 2 are shown in Table 3. For the suboptimal arrangement, $s_A = 6$ and the s_{ij}^A values for the interaction contrast vectors **12**, **13** and **23** are all ± 6. This is due to the fact that, in any of the four blocks of six runs defined by the row factor, all runs have the same sign for the contrast vectors of these interactions. This implies that these interactions are completely confounded with the blocks defined by the rows, and that the row effects and these three interaction effects could not be estimated separately if the suboptimal row-column arrangement were used in practice. For the **14**, **24** and **34** interactions, the s_{ij}^A values for the interaction contrast vectors are all ± 2. For this reason, the corresponding interaction effects are partially confounded with the rows. Therefore, considering the first blocking factor only, these interaction effects could be estimated if the suboptimal row-column arrangement were used in practice.

For the suboptimal row-column arrangement in Table 3, we also observe that $s_B = 4$. The only s_{ij}^B values of ± 4 occur for the **14** interaction contrast vector. Because there are eight experimental runs in each column, the confounding between the interaction contrast vector **14** and the columns is not complete. As a result, considering only the second blocking factor, the interaction effect between the first and the fourth factor would be estimable if the suboptimal row-column arrangement were used. All other s_{ij}^B values are zero, indicating that there is no confounding at all between the other two-factor interaction contrast vectors and the columns.

The optimal row-column arrangement in Table 3 has $s_A = 2$ and $s_B = 0$. As a result, that arrangement involves a limited amount of confounding between the two-factor interactions and the rows, and no confounding at all between the interactions and the columns. Therefore, the optimal row-column arrangement offers substantially more information concerning the interactions than the suboptimal one.

The s_A and s_B values quantify the severity of the worst type of the confounding of the treatment factors' interactions with the blocks. To distinguish among arrangements with equal s_A or s_B values, some measure of the total confounding is required as well. A interesting option for such a measure is based on the mixed-type word count introduced in the literature by Cheng and Wu (2002) for finding blocking schemes in scenarios involving a single blocking factor. The mixed-type word count was also used by Schoen et al. (2013, 2019) for problems involving one blocking factor only, and by Vo-Thanh et al. (2019) to identify row-column arrangements of small treatment designs using a complete enumeration approach. When focusing on orthogonal blocking patterns, the most important mixed-type word counts quantify the confounding of the two-factor interactions with the first blocking factor (i.e., with the rows) and with the second blocking factor (i.e., with the columns). We denote these words counts by A_3^r and A_3^c. Vo-Thanh et al. (2019) use the sum $A_3^{r,c} = A_3^r + A_3^c$ as a measure of the total amount of confounding between the two-factor interactions and the blocks. Row-column designs with low $A_3^{r,c}$ values are preferred, because, for these designs, there is little confounding between the interactions and the two blocking factors. Ideally, the $A_3^{r,c}$ value is zero, in which case the two-factor interactions are orthogonal to both blocking factors and there is no confounding between the two-factor interaction effects and the blocks.

One important issue with the A_3^r and A_3^c values is that they are not linear functions of the decision

variables a_{ij} and b_{ij}. In contrast, the elements of the matrices $\mathbf{S}_A$ and $\mathbf{S}_B$ are linear functions of a_{ij} and b_{ij}. For this reason, in this paper, we quantify the confounding between the two-factor interactions, on the one hand, and the rows and columns, on the other hand, using the matrices $\mathbf{S}_A$ and $\mathbf{S}_B$. In so doing, we extend the approach of Sartono et al. (2015) and Vo-Thanh et al. (2018) to the case of two blocking factors. Row-column arrangements for which $\mathbf{S}_A$ and $\mathbf{S}_B$ are zero matrices have zero A_3^r and A_3^c values, and vice versa. Similarly, row-column arrangements for which the entries of $\mathbf{S}_A$ and $\mathbf{S}_B$ are small in absolute value generally have small A_3^r and A_3^c values. The methods we use to identify good row-column arrangements in this paper minimize the absolute values of all entries of $\mathbf{S}_A$ and $\mathbf{S}_B$. More specifically, we first minimize the maximum absolute value of the elements of these matrices. Next, we minimize the sum of the absolute values of their elements. In doing so, we prioritize the avoidance of any severe confounding between the treatment factors' interactions and the blocks. Next, we try to minimize the remaining, less severe, confounding.

For the viability example, we enumerated all possible ways to arrange the given treatment design of Table 2 in four rows and three columns using the algorithm in Schoen et al. (2010). This resulted in 28,591 non-isomorphic row-column arrangements. Forty-five of these arrangements have an A_3^r value of 2/3 and an A_3^c value of zero. These 45 designs minimize the mixed-type word count $A_3^{r,c} = A_3^r + A_3^c$ and are optimal in terms of this count. The optimal row-column arrangement in Table 2 is one of these 45 arrangements. Because of the zero A_3^c value, the design allows the interaction effects to be estimated independently from the second blocking factor's effects, i.e., the column effects. The nonzero A_3^r value means that the interaction effects are confounded to some extent with the first blocking factor's effects, i.e., the row effects.

4 Methodology

In this section, we propose two different strategies to search for row-column arrangements of a given two-level factorial treatment design $\mathbf{X}$. Regardless of the strategy, the row-column arrangements should possess the following characteristics:

1. The main effects of the treatment factors should be orthogonal to the rows.
2. The confounding of the two-factor interactions with the rows should be minimal.
3. The main effects of the treatment factors should be orthogonal to the columns.
4. The confounding of the two-factor interactions with the columns should be minimal.
5. The rows and columns should be orthogonal to each other.

The two proposed strategies extend the mixed integer linear programming approach of SSG in two different ways. The first strategy is a sequential approach suitable when the confounding of the two-factor interactions with one of the two blocking factors is of a greater concern than the confounding with the other blocking factor. Without loss of generality, we assume that the blocking factor corresponding to the rows of the row-column design is the factor of greater concern. The second strategy is a simultaneous approach to find row-column arrangements when the confounding with both blocking factors is of equal concern.

The fact that we use minimum or nearly minimum G- and G_2-aberration strength-2 orthogonal treatment designs as well as strength-3 orthogonal treatment designs as an input to our approaches for finding row-column arrangements implies that all our row-column arrangements allow a main-effects model in the treatment factors and the blocking factors to be estimated with maximum precision. It also ensures there is as little aliasing as possible between the main effects and the second-order interaction effects of the treatment factors, and, given the amount of aliasing between the treatment factors' main effects and interactions, it also minimizes the confounding between the blocking factors and the second-order interactions of the treatment factors. The two strategies we propose below are intended to minimize the latter kind of confounding.

4.1 Sequential approach

4.1.1 Step 1

In the first step of the sequential approach, we arrange the given two-level treatment design $\mathbf{X}$ in a rows using the mixed integer linear programming approach of SSG, which was intended for finding orthogonal

blocking arrangements for problems involving one blocking factor. The resulting arrangement satisfies the goals (1) and (2).

To minimize the aliasing of the two-factor interactions with the rows, the approach of SSG sequentially minimizes the maximum absolute value of all elements of $\mathbf{S}_A$,

$$s_A = \max\{\left|s_{ik}^A\right|, i = 1, \ldots, q; k = 1, \ldots, a\},$$

and the sum of the absolute values of all elements of $\mathbf{S}_A$,

$$\gamma = \sum_{i=1}^{q}\sum_{k=1}^{a}\left|s_{ik}^A\right|.$$

The sequential minimization of s_A and γ is intended to ensure that no two-factor interaction is strongly confounded with the rows, and that, subsequently, all remaining confounding between the two-factor interactions and the rows is minimized.

Since linear programming approaches cannot deal with absolute values, we define the auxiliary non-negative variables s_{ik}^{A+} and s_{ik}^{A-} for each element s_{ik}^A of $\mathbf{S}_A$. The variable s_{ik}^{A+} equals s_{ik}^A if s_{ik}^A is positive, and zero otherwise. The variable s_{ik}^{A-} equals $-s_{ik}^A$ if s_{ik}^A is negative, and zero otherwise. Therefore, the variables s_{ik}^{A+} and s_{ik}^{A-} satisfy the equality

$$s_{ik}^A = s_{ik}^{A+} - s_{ik}^{A-}.$$

When expressed in terms of s_{ik}^{A+} and s_{ik}^{A-}, the secondary objective, γ, is

$$\gamma = \sum_{i=1}^{q}\sum_{k=1}^{a}(s_{ik}^{A+} + s_{ik}^{A-}).$$

Sequentially minimizing two objectives is known as pre-emptive goal programming or lexicographic goal programming in operations research. We implement our sequential minimization by assigning a large weight, M, to our primary objective, s_A, and a weight of one to our secondary objective, γ. This leads to the following linear optimization model for Step 1 of our sequential approach:

$$\min f = Ms_A + \gamma = Ms_A + \sum_{i=1}^{q}\sum_{k=1}^{a}(s_{ik}^{A+} + s_{ik}^{A-}), \tag{2}$$

subject to

$$\sum_{j=1}^{N} w_{ji}a_{jk} - s_{ik}^{A+} + s_{ik}^{A-} = 0, i = 1, \ldots, q; k = 1, \ldots, a, \tag{3}$$

$$0 \le s_{ik}^{A+} \le s_A, i = 1, \ldots, q; k = 1, \ldots, a, \tag{4}$$

$$0 \le s_{ik}^{A-} \le s_A, i = 1, \ldots, q; k = 1, \ldots, a, \tag{5}$$

$$\mathbf{X}^T\mathbf{A} = \mathbf{0}_{n\times a}, \tag{6}$$

$$\mathbf{1}_N^T\mathbf{A} = (N/a)\mathbf{1}_a^T, \tag{7}$$

$$\mathbf{A}\mathbf{1}_a = \mathbf{1}_N, \tag{8}$$

$$a_{ij} \in \{0, 1\}, i = 1, \ldots, N; j = 1, \ldots, a. \tag{9}$$

In the linear optimization model, Constraints (3)–(5) define the variables s_{ik}^{A+}, s_{ik}^{A-} and s_A required to calculate the weighted objective function in Equation (2), using linear expressions. Constraint (6) states that only orthogonal blocking arrangements are allowed, i.e., blocking arrangements in which the treatment factors' main effects are orthogonal to the rows. Constraint (7) ensures that each of the a columns of $\mathbf{A}$ contains N/a treatments (in other words, that each row of the row-column arrangement has N/a runs), and Constraint (8) ensures that every treatment is assigned to exactly one row. In these constraints, the vectors $\mathbf{1}_N$ and $\mathbf{1}_a$ are vectors of ones of dimension N and a, respectively. Finally, the binary nature of the matrix $\mathbf{A}$, which assigns the treatments to the rows, is imposed by Constraint (9), in which a_{ij} represents the element in the ith row and jth column of $\mathbf{A}$.

All decision variables in this linear optimization model are integer for two-level treatment designs, so that the model belongs to the class of integer linear programming models. The first goal we try to achieve, goal (1), is enforced by Constraint (6). Goal (2), is achieved by minimizing the linear program's objective function in Equation (2).

4.1.2 Step 2

Step 2 of the sequential approach starts from the optimal arrangement of the treatment design $\mathbf{X}$ in a rows produced by Step 1 and arranges the treatment design $\mathbf{X}$ in b columns as well, while leaving the arrangement in rows unchanged. Apart from one additional constraint, the linear optimization model in Step 2 has exactly the same structure as that in Step 1. The additional constraint in Step 2 ensures that the two blocking factors (i.e., the row factor and the column factor) are orthogonal to each other. This is necessary for the blocking factors to be crossed.

Denoting the auxiliary variables to model the absolute value of each element s_{ik}^{B} of the matrix $\mathbf{S}_B$ by s_{ik}^{B+} and s_{ik}^{B-}, the optimization model needed in Step 2 of the sequential approach is as follows:

$$\min f = Ms_B + \sum_{i=1}^{q}\sum_{k=1}^{b}(s_{ik}^{B+} + s_{ik}^{B-}), \tag{10}$$

subject to

$$\sum_{j=1}^{N} w_{ji}b_{jk} - s_{ik}^{B+} + s_{ik}^{B-} = 0, i = 1,\ldots,q; k = 1,\ldots,b, \tag{11}$$

$$0 \le s_{ik}^{B+} \le s_B, i = 1,\ldots,q; k = 1,\ldots,b, \tag{12}$$

$$0 \le s_{ik}^{B-} \le s_B, i = 1,\ldots,q; k = 1,\ldots,b, \tag{13}$$

$$\mathbf{X}^T\mathbf{B} = \mathbf{0}_{n\times b}, \tag{14}$$

$$\mathbf{A}_{\text{opt}}^T\mathbf{B} = (N/ab)\mathbf{J}_{a\times b}, \tag{15}$$

$$\mathbf{1}_N^T\mathbf{B} = (N/b)\mathbf{1}_b^T, \tag{16}$$

$$\mathbf{B}\mathbf{1}_b = \mathbf{1}_N, \tag{17}$$

$$b_{ij} \in \{0,1\}, i = 1,\ldots,N; j = 1,\ldots,b. \tag{18}$$

The linear optimization model in this step clearly also utilizes pre-emptive goal programming. This time, this is to prioritize the minimization of s_B. Constraints (11)–(13) define all the variables needed to calculate the objective function value in Equation (10). Constraint (14) ensures that the main effects of the treatment factors are all orthogonal to the columns. Constraint (15) is the new constraint which guarantees that the row blocking factor and the column blocking factor are orthogonal to each other. In that constraint, the matrix $\mathbf{A}_{\text{opt}}$ corresponds to the optimal row arrangement identified in Step 1, and the matrix $\mathbf{J}_{a\times b}$ represents the unit matrix of dimension $a \times b$. Constraints (16)–(18) ensure that the matrix $\mathbf{B}$ is binary, that every treatment is assigned to exactly one column of the design and that every column of the design contains N/b treatments. In Constraint (18), b_{ij} represents the element in row i and column j of the matrix $\mathbf{B}$.

Note that, in Step 2 of the sequential approach, the matrix $\mathbf{A}_{\text{opt}}$, which indicates how the treatments are assigned to the a rows of the row-column design, is given. So, in the linear program defined by Equations (10)–(18), the elements of $\mathbf{A}_{\text{opt}}$ are input parameters rather than decision variables, and all constraints are linear in the decision variables.

4.2 Simultaneous approach

In this section, we propose three different optimization models to construct row-column designs when the confounding of the two-factor interactions with the two blocking factor is of equal concern. The first two of these models directly aim at optimizing the assignment matrices $\mathbf{A}$ and $\mathbf{B}$ for the given treatment design $\mathbf{X}$. This necessitates an additional constraint that enforces the orthogonality between the rows and the columns of the row-column arrangement. The first optimization model involves a quadratic constraint that ensures the orthogonality between the rows and the columns. The second optimization model involves a linearization

of the quadratic constraint. The third optimization model avoids the extra orthogonality constraint by redefining the row-column arrangement problem as a permutation problem. In that model, the blocking structure is predefined, so that alternative row-column arrangements are represented as permutations of the treatment design $\mathbf{X}$. All three optimization models constitute a simultaneous approach that tackles the goals (1)–(5) at the same time.

4.2.1 Simultaneous approach 1: A quadratic model

In this section, we describe our first optimization model to find row-column arrangements when the confounding with both blocking factors is of equal concern. The main goal is to find the two blocking matrices $\mathbf{A}$ and $\mathbf{B}$ that result in minimal confounding between the two-factor interaction effects, on the one hand, and the rows and the columns, on the other hand. A technical constraint when seeking the optimal $\mathbf{A}$ and $\mathbf{B}$ matrices is that these two matrices should be orthogonal to each other.

Achieving the goals (1), (3) and (5) is ensured by entering them as constraints in the optimization model. The goals (2) and (4) are dealt with in the optimization model's objective function. In the three models we present for the simultaneous approach, the objective function expresses our intention to make the two confounding matrices $\mathbf{S}_A$ and $\mathbf{S}_B$ as small as possible simultaneously. In order to achieve this goal, we first minimize the maximum absolute value of all elements of the matrices $\mathbf{S}_A$ and $\mathbf{S}_B$,

$$s_{AB} = \max\{\left|s_{ij}^A\right|, \left|s_{ik}^B\right|, i = 1, \ldots, q, j = 1, \ldots, a, k = 1, \ldots, b\}.$$

Next, we also minimize the sum of the absolute values of all elements of the matrices $\mathbf{S}_A$ and $\mathbf{S}_B$,

$$\gamma_{AB} = \sum_{i=1}^{q}\sum_{j=1}^{a}\left|s_{ij}^A\right| + \sum_{i=1}^{q}\sum_{k=1}^{b}\left|s_{ik}^B\right|.$$

As in the sequential approach in Section 4.1, we implement the sequential minimization of s_{AB} and γ_{AB} using pre-emptive goal programing. Also, we again use the auxiliary variables s_{ik}^{A+}, s_{ik}^{A-}, s_{ik}^{B+} and s_{ik}^{B-} to deal with the absolute values of the elements of $\mathbf{S}_A$ and $\mathbf{S}_B$. We therefore calculate the sum of all of the absolute values of the elements of $\mathbf{S}_A$ and $\mathbf{S}_B$ as

$$\gamma_{AB} = \sum_{i=1}^{q}\sum_{k=1}^{a}(s_{ik}^{A+} + s_{ik}^{A-}) + \sum_{i=1}^{q}\sum_{k=1}^{b}(s_{ik}^{B+} + s_{ik}^{B-})$$

in our simultaneous optimization model:

$$\min f = Ms_{AB} + \gamma_{AB} = Ms_{AB} + \sum_{i=1}^{q}\sum_{k=1}^{a}(s_{ik}^{A+} + s_{ik}^{A-}) + \sum_{i=1}^{q}\sum_{k=1}^{b}(s_{ik}^{B+} + s_{ik}^{B-}), \tag{19}$$

subject to

$$\sum_{j=1}^{N} w_{ji}a_{jk} - s_{ik}^{A+} + s_{ik}^{A-} = 0, i = 1, \ldots, q; k = 1, \ldots, a, \tag{20}$$

$$\sum_{j=1}^{N} w_{ji}b_{jk} - s_{ik}^{B+} + s_{ik}^{B-} = 0, i = 1, \ldots, q; k = 1, \ldots, b, \tag{21}$$

$$0 \leq s_{ik}^{A+} \leq s_{AB}, i = 1, \ldots, q; k = 1, \ldots, a, \tag{22}$$

$$0 \leq s_{ik}^{A-} \leq s_{AB}, i = 1, \ldots, q; k = 1, \ldots, a, \tag{23}$$

$$0 \leq s_{ik}^{B+} \leq s_{AB}, i = 1, \ldots, q; k = 1, \ldots, b, \tag{24}$$

$$0 \leq s_{ik}^{B-} \leq s_{AB}, i = 1, \ldots, q; k = 1, \ldots, b, \tag{25}$$

$$\mathbf{X}^T\mathbf{A} = \mathbf{0}_{n\times a}, \tag{26}$$

$$\mathbf{X}^T\mathbf{B} = \mathbf{0}_{n\times b}, \tag{27}$$

$$\mathbf{A}^T\mathbf{B} = (N/ab)\mathbf{J}_{a\times b}, \tag{28}$$
$$\mathbf{1}_N^T\mathbf{A} = (N/a)\mathbf{1}_a^T, \tag{29}$$
$$\mathbf{1}_N^T\mathbf{B} = (N/b)\mathbf{1}_b^T, \tag{30}$$
$$\mathbf{A}\mathbf{1}_a = \mathbf{1}_N, \tag{31}$$
$$\mathbf{B}\mathbf{1}_b = \mathbf{1}_N, \tag{32}$$
$$a_{ij} \in \{0,1\}, i = 1,\ldots,N; j = 1,\ldots,a, \tag{33}$$
$$b_{ij} \in \{0,1\}, i = 1,\ldots,N; j = 1,\ldots,b. \tag{34}$$

Constraints (20)–(25) define all the variables needed to calculate the objective function value in Equation (19). Constraints (26) and (27) ensure that the main effects of the treatment factors are all orthogonal to the rows and the columns, respectively. Constraint (28) ensures that the row blocking factor and the column blocking factor are orthogonal to each other. Constraints (29) and (30) ensure that every row contains N/a treatments and that every column contains N/b treatments. Constraints (31) and (32) ensure that every treatment is assigned to exactly one row and to exactly one column, and Constraints (33) and (34) ensure that the matrices $\mathbf{A}$ and $\mathbf{B}$ are binary.

In the optimization model defined by Equations (19)–(34), Constraint (28) is quadratic, because it involves products of decision variables, namely the elements of the binary matrices $\mathbf{A}$ and $\mathbf{B}$. This is in contrast with Constraint (15) in Step 2 of the sequential approach, where the matrix $\mathbf{A}$ was fixed after the sequential approach's Step 1 and the matrix $\mathbf{B}$ was the only one to be optimized.

4.2.2 Simultaneous approach 2: The linearized quadratic model

Generally, solving optimization models involving quadratic constraints takes more computing time than solving models involving only linear constraints. It is, therefore, useful to try to replace quadratic constraints with linear ones.

In the case of Constraint (28), where the decision variables are binary, it is indeed possible to replace the quadratic expression with several linear constraints. To see this, note first that the original quadratic constraint is equivalent to

$$\sum_{k=1}^{N} a_{ki}b_{kj} = \frac{N}{ab},$$

for each row i and each column j of the row-column design. In the second simultaneous approach, we replace this quadratic expression by a new constraint,

$$\sum_{k=1}^{N} c_{ijk} = \frac{N}{ab}, \tag{35}$$

for each row i and each column j. The new constraint involves a new decision variable c_{ijk}, which we define as

$$c_{ijk} = a_{ki}b_{kj}.$$

The new decision variable is a product of two binary variables a_{ki} and b_{kj}. Consequently, it should also be binary. More specifically, c_{ijk} should take the value 1 if both a_{ki} and b_{kj} are 1, and zero otherwise. Now, instead of calculating c_{ijk} as a product of a_{ki} and b_{kj}, it can also be determined by using the following set of linear inequality constraints:

$$c_{ijk} \le a_{ki}, i = 1,\ldots,a; j = 1,\ldots,b; k = 1,\ldots,N, \tag{36}$$
$$c_{ijk} \le b_{kj}, i = 1,\ldots,a; j = 1,\ldots,b; k = 1,\ldots,N, \tag{37}$$
$$c_{ijk} \ge a_{ki} + b_{kj} - 1, i = 1,\ldots,a; j = 1,\ldots,b; k = 1,\ldots,N, \tag{38}$$
$$c_{ijk} \ge 0, i = 1,\ldots,a; j = 1,\ldots,b; k = 1,\ldots,N. \tag{39}$$

Given that c_{ijk} is non-negative, Inequalities (36) and (37) ensure that c_{ijk} takes the value zero when a_{ki} or b_{kj} are zero. Inequality (38) ensures that c_{ijk} takes the value one when a_{ki} and b_{kj} are both one. The crucial

Table 4: Creation of the new variable c_{ijk} from a_{ki} and b_{kj} by using Inequalities (36)–(39).

a_{ki}	b_{kj}	$a_{ki}+b_{kj}-1$	c_{ijk}
0	0	-1	0
0	1	0	0
1	0	0	0
1	1	1	1

role played by the sum $a_{ki}+b_{kj}-1$ in Inequality (38) is clarified in the final column of Table 4. That table shows all possible combinations of a_{ki} and b_{kj} values, as well the corresponding values of $a_{ki}+b_{kj}-1$ and c_{ijk}. The table allows us to verify that Constraints (36)–(39) do a good job at reproducing the value of the product $c_{ijk}=a_{ki}b_{kj}$, even though they do not involve products of a_{ki} and b_{kj} values.

It is clear that replacing the quadratic constraint in Equation (28) by Constraints (35)–(39) in the optimization model defined by Equations (19)–(34) results in a new optimization model that has the same optimal solution. A key difference between the new model and the original one is that the former only involves linear constraints, which is generally considered to be an advantage, despite the fact that the new formulation involves a larger number of constraints as well as a larger number of decision variables.

4.2.3 Simultaneous approach 3: A permutation-based model

In this section, we reformulate the problem of finding an optimal row-column arrangement as a permutation problem. Rather than optimizing the binary blocking matrices $\mathbf{A}$ and $\mathbf{B}$ from scratch, while ensuring that the corresponding blocking structure (the pattern of the rows and the columns) is orthogonal, the permutation problem formulation considers the blocking structure as given. Finding an optimal row-column arrangement of a treatment design then comes down to assigning the N treatments to the N positions in the predefined blocking structure. Therefore, we have to find a permutation of all N treatments, where the treatment appearing first in the permutation is assigned to the first position in the blocking structure (first experimental run at the first level of the first blocking factor and the first level of the second blocking factor), the treatment appearing second is assigned to the second position, etc. The treatment appearing last in the permutation is assigned to the last position in the blocking structure (last experimental run at the ath level of the first blocking factor and the bth level of the second blocking factor).

Every permutation of a set of N objects can be represented by a permutation matrix $\mathbf{P}$, i.e., an N-dimensional binary square matrix, involving exactly one entry of 1 in every row and in every column. For a given treatment design $\mathbf{X}$ with interaction contrast matrix $\mathbf{W}$ and a given orthogonal blocking structure $[\mathbf{A}\ \mathbf{B}]$, the confounding matrices $\mathbf{S}_A$ and $\mathbf{S}_B$ can be expressed in terms of the permutation matrices as well: $\mathbf{S}_A=\mathbf{W}^T\mathbf{P}\mathbf{A}$ and $\mathbf{S}_B=\mathbf{W}^T\mathbf{P}\mathbf{B}$. Similarly, the conditions that the main effects of the treatment factors should be orthogonal to the rows and the columns of the row-column design can be reformulated as $\mathbf{X}^T\mathbf{P}\mathbf{A}=\mathbf{0}_{n\times a}$ and $\mathbf{X}^T\mathbf{P}\mathbf{B}=\mathbf{0}_{n\times b}$, respectively. We denote the element in row i and column j of the permutation matrix $\mathbf{P}$ by p_{ij}. This element takes the value 1 if the ith treatment in $\mathbf{X}$ is assigned to the jth position in the blocking structure. The integer linear programming model based on the permutation matrix is then as follows:

$$\min f = Ms_{AB}+\gamma_{AB} = Ms_{AB}+\sum_{i=1}^{q}\sum_{k=1}^{a}(s_{ik}^{A+}+s_{ik}^{A-})+\sum_{i=1}^{q}\sum_{k=1}^{b}(s_{ik}^{B+}+s_{ik}^{B-}), \tag{40}$$

subject to

$$\sum_{j=1}^{N}\Big(\sum_{m=1}^{N}w_{mi}p_{mj}\Big)a_{jk}-s_{ik}^{A+}+s_{ik}^{A-}=0, i=1,\ldots,q; k=1,\ldots,a, \tag{41}$$

$$\sum_{j=1}^{N}\Big(\sum_{m=1}^{N}w_{mi}p_{mj}\Big)b_{jk}-s_{ik}^{B+}+s_{ik}^{B-}=0, i=1,\ldots,q; k=1,\ldots,b, \tag{42}$$

$$0\le s_{ik}^{A+}\le s_{AB}, i=1,\ldots,q; k=1,\ldots,a, \tag{43}$$

$$0\le s_{ik}^{A-}\le s_{AB}, i=1,\ldots,q; k=1,\ldots,a, \tag{44}$$

$$0 \leq s_{ik}^{B+} \leq s_{AB}, i = 1, \ldots, q; k = 1, \ldots, b, \tag{45}$$

$$0 \leq s_{ik}^{B-} \leq s_{AB}, i = 1, \ldots, q; k = 1, \ldots, b, \tag{46}$$

$$\mathbf{X}^T\mathbf{PA} = \mathbf{0}_{n\times a}, \tag{47}$$

$$\mathbf{X}^T\mathbf{PB} = \mathbf{0}_{n\times b}, \tag{48}$$

$$\mathbf{P1}_N = \mathbf{1}_N, \tag{49}$$

$$\mathbf{1}_N^T\mathbf{P} = \mathbf{1}_N^T, \tag{50}$$

$$p_{ij} \in \{0, 1\}, i, j = 1, \ldots, N. \tag{51}$$

The objective function in the new formulation is exactly the same as that in the two other models for the simultaneous approach in Sections 4.2.1 and 4.2.2. Constraints (41)–(46) in the new formulation define the various components of the objective function. The differences between these constraints and those in the previous formulations is that Constraints (41) and (42) now make use of the elements of the permutation matrix, and that $\mathbf{A}$ and $\mathbf{B}$ are now given matrices defining two blocking factors that are orthogonal to each other rather than matrices with decision variables. More specifically, $\mathbf{A} = \mathbf{I}_a \otimes \mathbf{1}_{N/a}$ and $\mathbf{B} = \mathbf{1}_a \otimes \mathbf{I}_b \otimes \mathbf{1}_{N/(ab)}$, where $\mathbf{I}_a$ and $\mathbf{I}_b$ are identity matrices of dimension a and b, respectively. Constraints (47) and (48) ensure that the treatment factors' main effects are orthogonal to the rows and columns, respectively. Finally, constraints (49)–(51) define the technical properties of the permutation matrix $\mathbf{P}$. The final constraint enforces $\mathbf{P}$ to be a binary matrix, and Constraints (49) and (50) ensure that there is a one in every row and in every column of the permutation matrix.

A key difference between the optimization model defined by Equations (40)–(51) and the models in Sections 4.2.1 and 4.2.2 is that the elements of the matrices $\mathbf{A}$ and $\mathbf{B}$ are given, so that the permutation-based approach does not involve quadratic constraints.

5 Computational results

In this section, we apply the four optimization models, one for the sequential approach from Section 4.1 and three for the simultaneous approach from Section 4.2, to three different kinds of problem. First, we study the arrangement of 24-run orthogonal two-level treatments designs in four rows and three columns. Next, we study the arrangement of 64-run orthogonal two-level designs in four rows and four columns. Finally, we study arrangements of 72-run orthogonal two-level designs in three rows and three columns. We selected these three specific kinds of problem because benchmark results are available from the literature. In particular, Vo-Thanh et al. (2019) used a complete enumeration to identify good row-column arrangements of strength-2 24-run two-level designs and strength-3 64- and 72-run two-level designs. The sequential and simultaneous optimization approaches presented here are much more generally applicable than the complete enumeration approach of Vo-Thanh et al. (2019), but we believe that demonstrating that these approaches produce the same quality of designs as the complete enumeration approach is a powerful proof of concept.

In all our comparisons, we pay attention to the quality of the row-column arrangements produced as well as the required computing time. For all of the cases studied, we set the value of M in the pre-emptive goal programming to 10,000. We performed all computations under Windows 7 (64-bit) on a Intel core i7-3770 PC with a 3.4GHz CPU for the 24-run designs and with a 2.6GHz CPU for the other designs, and an internal memory of 16 GB, using MATLAB 2012b along with CPLEX version 12.6.1. We used a time limit of 10,000 seconds for each approach for each problem tackled.

Following Vo-Thanh et al. (2019), we assume in the comparisons we make in this section that the confounding of two-factor interactions with the row factor and with the column factor is of equal concern to the experimenter. Therefore, our evaluation of the different optimization approaches is based on the objective function in Equation (19) (which is identical to that in Equation (40)). It should be pointed out, however, that Vo-Thanh et al. (2019) used different objective functions, based on the mixed-type words counts mentioned in Section 3.2.

5.1 24-run designs

For our computational experiments involving 24-run two-level designs, we use the two-level orthogonal treatment designs from the W_2- and W_3-optimal row-column arrangements identified by Vo-Thanh et al. (2019). This is because these designs perform very well in terms of the G- or G_2-aberration criterion, and because we can use the row-column arrangements of Vo-Thanh et al. (2019) as benchmarks. Our use of minimum or nearly minimum G- or G_2-aberration orthogonal treatment designs implies that the row-column arrangements we obtain allow the treatment factors' main effects to be estimated independently from each other, from the rows and from the columns. In addition, the aliasing between the treatment factors' second-order interactions and their main effects is minimal, as well as their confounding with the rows and the columns. In total, we consider 17 different 24-run two-level treatment designs. The smallest design involves four factors, while the two largest designs involve 13 factors. The four-factor design is the one shown in Table 2.

The objective function values of the row-column arrangements of the 24-run designs obtained by the four optimization approaches from Section 4 are listed in Table 5. The table's first column identifies the designs arranged in rows and columns. The designs' IDs are of the form $n.i$, where n denotes the number of two-level treatment factors and i is a label distinguishing designs with the same numbers of factors. The next three columns show the computing times required by the sequential approach, the objective function values produced by it, and the $A_3^{r,c}$ values quantifying the confounding between the treatment factors' interactions and both blocking factors in the resulting row-column arrangements. The next column shows the objective function values produced by the quadratic programming model, the linearized quadratic programming model and the permutation-based model, and the $A_3^{r,c}$ values of the corresponding row-column arrangements. Remarkably, each of the three models for the simultaneous approach resulted in the same value for the objective function and the same $A_3^{r,c}$ value except for treatment design 10.2. For that case, the $A_3^{r,c}$ value for the row-column arrangement of treatment design 10.2 obtained from the quadratic model and from the permutation-based model is 16.17, while the $A_3^{r,c}$ value obtained from the linearized quadratic model is 16.61. All of the objective function values are optimal, because the linearized quadratic model and the permutation-based model were both solved to optimality well within the computing time limit of 10,000 seconds for each treatment design studied. The quadratic model returned the same objective function values as the other models. In nine of the 17 cases tackled with the quadratic model approach, CPLEX confirmed the optimality of the row-column arrangement. In the other eight cases, the computing time limit was reached before the CPLEX solver was able to confirm the optimality of the solution. The computing times for the three simultaneous optimization models are shown in Table 5 as well. The table's final column shows the objective values of the benchmark designs, i.e., the W_2- and W_3-optimal row-column arrangements identified by Vo-Thanh et al. (2019).

The results for treatment design 4.1 in the first line of the table correspond to the optimal row-column arrangement in Table 2 and the optimal $\mathbf{S}_A$ and $\mathbf{S}_B$ matrices in Table 3. The maximum absolute value of an element of $\mathbf{S}_A$ and $\mathbf{S}_B$ for that row-column arrangement is 2, and, in total, there are 24 occurrences of the values $+2$ or -2, resulting in an objective function value of $2 \times 10,000 + 24 \times 2 = 20,048$. In contrast, the sub-optimal arrangement in Table 2 results in the sub-optimal $\mathbf{S}_A$ and $\mathbf{S}_B$ matrices in Table 3. The maximum absolute value of an element of $\mathbf{S}_A$ and $\mathbf{S}_B$ for the sub-optimal row-column arrangement is 6, and, in total, there are 12 occurrences of the values $+6$ or -6, two occurrences of the values $+4$ or -4 and 12 occurrences of the values $+2$ or -2. The objective function value for this arrangement is therefore of $6 \times 10,000 + 12 \times 6 + 2 \times 4 + 12 \times 2 = 60,104$. This arrangement has been included for illustration only; it is not a result found be any of the optimization models.

The three simultaneous optimization models result in the best possible objective function value for each two-level treatment design considered. That is not always the case with the sequential approach: for eight- and nine-factor treatment designs, and for the designs 7.1, 10.2 and 11.1, the sequential approach results in a larger value for the objective function. For treatment designs 7.1, 10.2 and 11.1, the objective function values obtained from the sequential approach are only 24, 16, and 24 units larger, respectively, than those obtained from the simultaneous approach. This indicates that the maximum absolute elements of the matrices $\mathbf{S}_A$ and $\mathbf{S}_B$ are the same for both approaches, and that only the sum of the absolute elements, γ_{AB}, differs to some extent. For treatment designs 8.1, 8.2, 9.1 and 9.2, the objective function value obtained from the sequential approach is about $20,000 = 2 \times M$ units larger than that obtained from the simultaneous approach. This indicates that the maximum absolute element of the matrices $\mathbf{S}_A$ and $\mathbf{S}_B$ is different for both approaches: regardless of the exact model used, the simultaneous approach was able to identify row-column

arrangements whose s_{AB} values are two units smaller than those of the row-column arrangements produced by the sequential approach. For all treatment designs with 4–6, 12 and 13 factors, the sequential approach identifies row-column arrangements with the same values for the objective function as the simultaneous approach.

That the sequential approach does not always match the results produced by the simultaneous approach is logical: the sequential approach prioritizes the arrangement of the treatment design in rows, and, therefore, it may result in a poorer subsequent arrangement of the treatment design in columns. It should be pointed out, however, that the sequential approach is faster than the simultaneous approach (regardless of the model used), and that it produces competitive designs, with an s_{AB} value that is at most two units larger than that produced by the simultaneous approach. When comparing the designs from the sequential approach with the benchmark designs, we can see that their objective function values are alike, so that they possess the same s_{AB} values for each treatment design considered.

Comparing the row-column arrangements produced by the simultaneous approach and the benchmark row-column arrangements, we can see that their objective function values are identical for seven of the 17 treatment designs studied. For treatment designs 10.1, 10.2, 11.1, 11.2 and 13.2, the benchmark designs have a slightly higher objective function value. This indicates that the maximum absolute elements of the matrices $\mathbf{S}_A$ and $\mathbf{S}_B$ are the same for the designs produced by the simultaneous approach and the benchmark designs, and that only the sum of the absolute elements, γ_{AB}, differs to some extent. For treatment designs 7.1, 8.1, 8.2, 9.1 and 9.2, the differences in objective function values are about 20,000, indicating a difference of 2 in the value of s_{AB} for the row-column arrangements produced by the simultaneous approach and the benchmark row-column arrangements. It is clear, however, that the simultaneous approach leads to row-column arrangements with properties at least similar to those of the benchmark designs produced by the complete enumeration approach of Vo-Thanh et al. (2019).

To support this conclusion, we show the $A_3^{r,c}$ values of the row-column arrangements produced using our optimization approaches and the benchmark arrangements in Table 5. These values quantify the extent to which two-factor interaction effects are confounded with the rows and the columns. The benchmark designs score best in terms of the $A_3^{r,c}$ value, because they were selected based on that criterion. For ten of the 17 treatments designs, however, the simultaneous optimization models lead to row-column arrangements with the optimal $A_3^{r,c}$ value. The sequential approach produces row-column arrangements with an optimal $A_3^{r,c}$ value for 13 of the 17 treatment designs. For eight-factor and nine-factor treatment designs, there is a substantial difference in $A_3^{r,c}$ value between the benchmark row-column arrangements and those produced by the simultaneous approach. So, for eight- and nine-factor treatment designs, the difference between the optimization criterion used in the present paper and the criteria used in Vo-Thanh et al. (2019) is largest.

Of the three models we compared for the simultaneous approach, the linearized quadratic model is the fastest for the 17 treatment designs considered. The quadratic programming model is the slowest for each treatment design under consideration. For eight treatment designs, the quadratic programming model was unable to confirm that the solution it returned was indeed optimal. Allowing for more than 10,000 seconds of computing time would remedy this problem. However, the linearized quadratic model did not suffer from this problem and established the optimality of its solutions well within 10,000 seconds. Except for one case, this is also true for the permutation-based model. For this reason, we recommend against using the quadratic model, even though it involves fewer decision variables than the other two simultaneous optimization approaches, fewer constraints than the linearized quadratic programming approach and about as few constraints as the permutation-based approach. The numbers of decision variables and the numbers of constraints in the three simultaneous optimization models are shown in the columns labeled "Var" and "Con" in Table 5.

As a conclusion, our application of the sequential and simultaneous optimization approaches in the 24-run case has shown that the linearized quadratic model is the best simultaneous optimization model, followed by the permutation-based model. The quadratic programming model is not competitive in terms of computing time. Remarkably, in terms of solution quality, the sequential approach performs very well too for the smallest numbers of treatment factors and the largest numbers of treatment factors, even though that approach prioritizes one blocking factor over the other and the comparison we make in this section assumes that the confounding of two-factor interactions with either blocking factor is of equal concern. Due to its speed, we also recommend the sequential approach for small and large numbers of treatment factors.

Table 5: Results obtained when arranging 24-run two-level treatment designs involving 4–13 factors in four rows and three columns using the sequential approach and the three models for the simultaneous approach. Obj: objective function value; CT: computing time in seconds; $A_3^{r,c}$: $A_3^r + A_3^c$; Var: number of decision variables (simultaneous approach only); Con: number of constraints (simultaneous approach only); QM: quadratic model; LQM: linearized quadratic model; PM: permutation-based model.

ID	Sequential approach			Simultaneous approach										Benchmark	
				Obj	$A_3^{r,c}$	QM			LQM			PM				
	CT	Obj	$A_3^{r,c}$			CT	Var	Con	CT	Var	Con	CT	Var	Con	Obj	$A_3^{r,c}$
4.1	0.25	20048	0.67	20048	0.67	447.32	253	217	7.27	541	1069	26.55	661	202	20048	0.67
5.1	0.53	40112	1.78	40112	1.78	10000	309	307	28.78	597	1159	69.59	717	293	40112	1.78
6.1	0.58	40168	2.67	40168	2.67	6358.49	379	418	22.06	667	1270	72.88	787	405	40168	2.67
6.2	0.59	40176	2.83	40176	2.83	1896.77	379	418	14.15	667	1270	36.77	787	405	40176	2.83
7.1	1.16	60304	5.44	60280	5.50	4635.45	463	550	11.84	751	1402	66.19	871	538	80280	5.11
7.2	0.44	40248	4.00	40248	4.00	3923.00	463	550	5.51	751	1402	38.47	871	538	40248	4.00
8.1	0.72	80392	7.06	60388	8.61	1939.83	561	703	10.47	849	1555	50.90	969	692	80392	7.06
8.2	0.78	80368	6.61	60412	9.67	10000	561	703	35.62	849	1555	162.49	969	692	80368	6.28
9.1	0.83	80520	10.33	60540	13.00	10000	673	877	15.58	961	1729	98.62	1081	867	80552	10.00
9.2	0.72	80480	9.11	60524	12.11	289.26	673	877	7.54	961	1729	36.47	1081	867	80496	8.78
10.1	0.80	80664	13.00	80664	13.00	10000	799	1072	277.96	1087	1924	346.60	1207	1063	80680	13.00
10.2	1.05	80720	16.00	80704	16.17/16.61	10000	799	1072	18.55	1087	1924	58.30	1207	1063	80744	16.00
11.1	1.22	80896	20.00	80872	20.67	10000	939	1288	20.19	1227	2140	53.15	1347	1280	80912	20.00
11.2	8.56	80992	25.00	80992	25.00	10000	939	1288	1551.49	1227	2140	2046.94	1347	1280	81000	25.00
12.1	11.39	81200	30.00	81200	30.00	10000	1093	1525	2171.92	1381	2377	10000	1501	1518	81200	30.00
13.1	0.77	81040	20.00	81040	20.00	110.78	1261	1783	1.50	1549	2635	8.80	1669	1777	81040	20.00
13.2	0.69	81056	20.00	81056	20.00	30.58	1261	1783	1.00	1549	2635	6.52	1669	1777	81080	20.00

Table 6: Results obtained when arranging strength-3 64- and 72-run two-level treatment designs involving 6–12 factors in four rows and four columns and three rows and three columns, respectively, using the sequential approach, the linearized quadratic model and the permutation-based model. Obj: objective function value; CT: computing time in seconds; LQM: linearized quadratic model; PM: permutation-based model.

Number of Runs	ID	Sequential approach		Simultaneous approach			
				LQM		PM	
		CT	Obj	CT	Obj	CT	Obj
64	6.1	2.29	0	482.14	0	3922.96	0
	7.1	0.73	0	227.34	0	21.40	0
	8.3	0.31	0	3.71	0	4.26	0
	9.1	0.37	0	8.10	0	15.27	0
	9.2	0.36	0	109.04	0	14.98	0
	10.1	0.28	0	3.56	0	14.81	0
	11.1	0.59	0	13.34	0	9.84	0
	11.2	80.25	40064	10.89	0	8.03	0
	11.3	0.20	0	3.40	0	10.23	0
	11.4	107.31	40128	12.46	0	13.04	0
	12.1	40.01	40128	2.57	0	7.89	0
	12.2	94.69	40192	12.95	0	8.44	0
72	6.1	1.09	0	60.37	0	1941.45	0
	7.1	88.67	0	10000	40016	10000	40104
	8.1	10000	40048	573.37	0	10000	40328
	9.1	1.11	0	135.88	0	5712.54	0
	10.1	0.92	0	14.62	0	6280.68	0
	11.1	1.09	0	52.57	0	43.41	0
	12.1	0.25	0	104.68	0	48.39	0

5.2 64-run and 72-run designs

In this section, we study the arrangement of 12 strength-3 64-run two-level treatment designs in four rows and four columns and of seven strength-3 72-run two-level treatment designs in three rows and three columns, using the sequential approach, the linearized quadratic model and the permutation-based model. We disregarded the quadratic model due to its poor computing times. We focus on scenarios where the optimal value of the objective functions for the sequential approach and the simultaneous approach is known to be zero. So, we study scenarios in which all main effects and all two-factor interaction effects can be made orthogonal to the two blocking factors. The optimal row-column arrangements for these scenarios correspond to the strength-3 64-run and 72-run mixed-level orthogonal designs of the types $\mathrm{OA}(64, 4^2 \times 2^n, 3)$ and $\mathrm{OA}(72, 3^2 \times 2^n, 3)$ identified by Vo-Thanh et al. (2019). All these row-column arrangements involve up to 12 treatment factors.

For eight of the 12 64-run treatment designs considered, the sequential approach, the linearized quadratic model and the permutation-based model lead to an optimal row-column arrangement, with a zero objective function value. For the four remaining treatment designs, the simultaneous optimization models also produce an optimal row-column arrangement, but the sequential approach does not. So, in these cases, the sequential approach is unable to arrange the rows and the columns orthogonally to all main effects and all two-factor interactions. The treatment designs for which the sequential approach does not result in a zero objective value have all been optimally arranged in rows and columns in less than 13 seconds by the linearized quadratic model approach, and in less than 14 seconds by the permutation-based approach. As a result, these particular treatment designs are not very hard to arrange in rows and columns. The exact objective function values and the required computing times for the twelve 64-run treatment designs are shown in the top part of Table 6. The permutation-based approach is faster than the linearized quadratic model approach in five of the 12 cases. For treatment design 6.1, however, the permutation-based approach is very slow compared to the linearized quadratic model approach. In terms of the computing time, the linearized quadratic model and the permutation-based model are close competitors for the 64-run designs.

For five of the seven treatment 72-run designs, the sequential approach, the linearized quadratic model approach and the permutation-based model approach succeeded in identifying an optimal row-column arrangement, with an objective function value of zero. In all of these cases, the sequential approach is the fastest. For treatment design 7.1, the simultaneous approach did not produce an optimal row-column arrangement within 10,000 seconds, while the sequential approach was able to find one in about 89 seconds. For treatment design 8.1, the sequential approach and the permutation-based model fail to find an optimal row-column arrangement within 10,000 seconds, while the linearized quadratic model does manage to identify one in less than 600 seconds. In total, the simultaneous approach fails to find two optimal row-column arrangements when the permutation-based model is used. The permutation-based model approach is therefore the poorest of the three approaches investigated in this section in terms of the solution quality for the 72-run designs. For treatment designs 6.1, 9.1, and 10.1, it is also very slow compared to the other two models. Whenever the permutation-based model yields an optimal row-column arrangement fast, the other two methods do not require much computing time either. The exact objective function values and the required computing times for the seven 72-run treatment designs are shown in the bottom part of Table 6.

6 Discussion

In this paper, we proposed several integer programming approaches to arrange a given orthogonal two-level treatment design in rows and columns. This is useful for experiments involving two crossed blocking factors. A major advantage of using integer programming is that, unless the solver is stopped prematurely by the user, it guarantees an optimal solution.

The first approach we presented is a sequential approach, which we originally intended to be used when the confounding of the two-factor interactions with one of the two blocking factors is more of a concern than the confounding with the other blocking factor. However, our computational results show that, for small and for large numbers of treatment factors, the row-column arrangements produced by the sequential approach are also optimal when the confounding of the two-factor interactions with both blocking factors is of equal concern, and that the sequential approach is generally very fast.

The second approach we present is a simultaneous approach which assumes that we are concerned about the confounding of the two-factor interactions with the first blocking factor as much as we are concerned about the confounding of the interactions with the second blocking factor. We describe three variants of the simultaneous approach, one of which, involving a quadratic programming model, requires considerably more computing time than the other two. The latter two variants do not involve quadratic constraints. The so-called linearized quadratic modeling variant is in most cases faster than the permutation-based model. The simultaneous approach outperforms the sequential approach in terms of solution quality for moderate numbers of factors.

We also explored a third kind of approach, in which we use the row-column arrangement produced by the sequential approach as input for the simultaneous approach. This led to very fast computing times for both the linearized quadratic model and the permutation-based model, provided that the sequential approach produces a solution within seconds. Whenever the sequential approach requires 10 seconds or more, using its output as an input for the linearized quadratic model and the permutation-based model slows the solution of these optimization models down. For a few treatment designs, it even causes the solution of the two models to hit the computing time limit. For the detailed computational results for the third kind of approach, we refer to the online supplement to this paper.

In the event we are concerned about the confounding of the two-factor interactions with the first blocking factor as much as we are concerned about the confounding of the interactions with the second blocking factor, our recommendation is to use the following procedure for configurations similar to ours:

1. Find a row-column arrangement for the treatment design under consideration using the sequential approach.

2. If the sequential approach produces an optimal solution within 10 seconds, use that solution as input for the linearized quadratic model.

3. If the sequential approach does not finish within 10 seconds, run the linearized quadratic model from scratch, without using a starting solution as input.

We end up recommending the linearized quadratic model rather than the permutation-based model, because the latter occasionally fails to converge to optimality within 10,000 seconds, even though it performs very well in the vast majority of the cases (especially when a high-quality solution from the sequential approach is used as input).

In this article, we applied the various optimization models to sets of 24-run, 64-run and 72-run designs, because high-quality benchmark row-column arrangements exist for these run sizes. We would like to emphasize, however, that both our sequential approach and our simultaneous approach are much more broadly applicable than demonstrated here. More specifically, the high-quality benchmark arrangements were obtained by searching through a complete enumeration of orthogonal arrays of the type $\mathrm{OA}(N, a \times b \times 2^n, t)$, while the new approaches presented here work on any single treatment design. This is especially attractive when high-quality treatment designs are readily available, while at the same time a complete enumeration of orthogonal arrays of the type $\mathrm{OA}(N, a \times b \times 2^n, t)$ is infeasible. For example, minimum G-aberration designs of strength 3 are known for 32, 40 and 48 runs. However, catalogs of orthogonal arrays of the type $\mathrm{OA}(N, a \times b \times 2^n, 3)$ for these run sizes only cover the following cases: (a) $\mathrm{OA}(32, 4 \times 4 \times 2^n, 3)$ for $n \leq 4$, (b) $\mathrm{OA}(48, 4 \times 3 \times 2^n, 3)$ for $n \leq 4$ and (c) $\mathrm{OA}(48, 6 \times 4 \times 2^n, 3)$ for $n \leq 2$. Any complete strength-2 catalog for $N \geq 32$ is computationally infeasible. Therefore, in these cases, it is attractive to start with a minimum G-aberration design and use our methodology to obtain a good row-column arrangement.

For all treatment designs considered in this article, an orthogonal row-column arrangement happened to exist. However, there are minimum G-aberration designs and minimum G_2-aberration designs for which no such row-column arrangements exist. To find the best non-orthogonal row-column arrangement for such designs, we would need to modify our integer programming formulations to some extent. For example, in the simultaneous approaches, we would have to remove the constraints $\mathbf{X}^T\mathbf{A} = \mathbf{0}_{n\times a}$ and $\mathbf{X}^T\mathbf{B} = \mathbf{0}_{n\times b}$ from the problem formulation and add the maximum absolute elements of the matrix products $\mathbf{X}^T\mathbf{A}$ and $\mathbf{X}^T\mathbf{B}$ to the objective function (in the same fashion as the maximum absolute elements of $\mathbf{W}^T\mathbf{A}$ and $\mathbf{W}^T\mathbf{B}$), as well as the sum of their absolute elements. To prioritize the minimization of the two maximum absolute elements of $\mathbf{X}^T\mathbf{A}$ and $\mathbf{X}^T\mathbf{B}$ and the two sums of absolute elements over the minimization of the corresponding values for the two-factor interactions, we need to give them a large weight in the objective function.

Finally, there are various ways in which the work we presented here can be generalized. First, while we focused on two-level treatment designs here, it is not very difficult to generalize the sequential and simultaneous approaches to deal with multi-level designs and mixed-level designs. These designs involve at least one factor that has more than two levels. Second, both our sequential and simultaneous approaches can be extended to deal with more than two crossed blocking factors as well. For instance, for three blocking factors instead of two, we need to optimize an $N \times c$ binary assignment matrix $\mathbf{C}$, which assigns the N runs to the c levels of the third blocking factor, in addition to the matrices $\mathbf{A}$ and $\mathbf{B}$, which assign the runs to the levels of the first two blocking factors. When optimizing $\mathbf{C}$, we should make sure that the three blocking factors are pairwise orthogonal. Any quadratic constraints arising from this requirement can be linearized using the methodology sketched in Section 4.2.2.

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