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Bi-objective mathematical model for optimal sequencing of two-level factorial designs

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Abstract. Conducting sequencing experiments with good statistical properties and low cost is a crucial challenge for both researchers and practitioners. The main reason for this challenge is the combinatorial nature of the problem and the possible conflicts among objectives. The problem was addressed by proposing a mathematical programming formulation aimed at generating minimum-cost run orders with the best statistical properties for 2^k full-factorial and fractional-factorial designs. The approach performance is evaluated using designs of up to 64 experiments with different levels of resolution. The results indicate that the approach can yield optimal or sub-optimal solutions, depending on the objectives established for a given design matrix.

1 Introduction

Among the various techniques and tools for improving quality and productivity, factorial Design of Experiments (DoE) has become particularly popular in companies' practices. Introduced by Fisher (1926), it consists of a combination of sequences of runs performed to describe an empirical relationship between a set of controlled variables (which are called factors) and one or more response variables (Bhowmik et al., 2015, Box, Hunter and Hunter, 2005, Fisher, 1926).

Textbooks about DoE report that the order of execution of factorial designs should be random, no systematic, as randomization of run orders can avoid bias in the estimates of the effects of interest. However, randomization can induce many changes in factors, which will eventually increase the experimentation cost (Hilow, 2013).

The response from a factorial experiment carried out in a time sequence may be affected by uncontrollable variables that are highly correlated with the time in which they occur. In such a situation, a possibility is to randomize the run order of the experiment. Another possibility is to use a systematic run order that is robust against time trends (Angelopoulos, Evangelaras and Koukouvinos, 2009, Adekeye and Kunert, 2006). Hilow (2013) argues that systematic run (i.e., non-randomized) experimentation presents two major problems: (1) Responses may be adversely affected by highly correlated or aliased unrelated factors with order of experimentation (i.e., time), where the conditions of experimental stages may not be uniform and where successively generated responses may be contaminated by this time trend, thus influencing effect estimates; (2) Certain sequences (i.e., run-time orders) of the factorial experiment can be costly, especially if the level of change between steps involves factors with expensive or levels difficult to vary.

Box, Hunter and Hunter (2005) point out the experimental error as one of the most important source of errors faced by an investigator. By using sound principles of experimental

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design, in particular, randomization, data can be generated and provide a better basis for deducing causality.

Two main research questions concerning DoE can be identified: optimal experiments and sequence run. Regarding optimal experiments, see Street and Burgess (2008), Aggarwal, Veena and Lin (2003), Galil and Kiefer (1980), and Dykstra (1971). Concerning sequence run, see Alonso et al. (2011) and Wilmut and Zhou (2011). Suen, Das and Midha (2013) show details of its construction. With respect to experiment execution order, which affects not only the cost of transition between runs, see Garroi, Goos and Sörensen (2009), Wang and Chen (1998), Wang and Jan (1995), Wang (1991), Cheng and Jacroux (1988), Draper and Stoneman (1968), and Daniel and Wilcoxon (1966). As for the design robustness, since estimates of the main effects and interactions along the runs may be susceptible to the lack of control, see Oprime, Pureza and Oliveira (2017), Bhowmik et al. (2017), Hilow (2013) and Correa, Grima, Pere and Tort-Martorell (2009)

The problem of obtaining run orders of experiments that combine good statistical properties and low cost (here referred to as the Experiment Sequencing Problem—ESP) was first studied by Draper and Stoneman (1968) and Dickinson (1974). These authors compute the cost of an experimental design as the number of changes in factor levels (setup cost), which increase when one experiment is followed by another. The quality of statistical properties is assessed by measuring the effects of trends on selected factors. For example, the effects of the linear time trend are strong when there is high correlation between the order in which runs are performed and one or more factors.

Despite the theoretical development that followed in this field, difficulties in obtaining experimental designs with good statistical properties and low cost still persist. The reason is that these two criteria may be conflicting. ESP is a combinatorial problem, which explains why the computational effort required for the complete enumeration of the run orders of experiments has severely limited the size of the problem that could be exactly solved in an exactly manner (Tsao and Liu, 2008, Joiner and Campbell, 1976, Dickinson, 1974, Draper and Stoneman, 1968, Daniel and Wilcoxon, 1966). Bhowmik et al. (2017) and Bhowmik et al. (2015) have proposed a method for obtaining minimally changed run orders in symmetric factorial experiments. For instance, the authors have shown that minimally changed run orders in factorial experiments are not unique. Thus, they have developed an exhaustive search procedure for generating all possible run orders in 2^{k-p} fractional factorial design with minimum factor change.

In this work, a mathematical method based on a mixed-integer 0–1 bi-objective optimization model that describes the ESP has been proposed. The model is used to generate two-level run orders of factorial experiments that are robust to the linear time trend with minimally changed run orders. The number of runs that are conducted in this study varies from 8 to 64 with different levels of resolution. For a range of regular DoEs, the run orders are provided in Table 2. In Table 3, systematic sequences of runs for irregular DoEs are shown, with exception of case 2, which is a regular matrix. These are examples of applications. The method can be applied to other DoE types, considering replicate cases and factor change. Therefore, in this paper, two-level factorial design with and without replication is considered.

This work was organized as follows: Section 2 describes the criteria used in sequencing factorial designs and literature reviews. Section 3 presents the proposed optimization model and the methodology used to solve it. Computational experiments are presented in Section 4, followed by conclusions and next steps in Section 5.

2 Criteria for systematic sequence of two-level factorial design

In a 2^k factorial design, the lower and upper levels of each factor are usually coded by minus and plus signs, respectively. An example of a three-factor design matrix (denoted as a, b

Run	a	b	c		y
1	–	–	–	1	y_1
2	+	–	–	a	y_2
3	–	+	–	b	y_3
4	+	+	–	ab	y_4
5	–	–	+	c	y_5
6	+	–	+	ac	y_6
7	–	+	+	bc	y_7
8	+	+	+	abc	y_8

Figure 1 *Design matrix for a* 2^3 *factorial experiment.*

and c) is presented in columns 2–4 of Figure 1. For any collection of k columns of such a matrix, each of the 2^k row vectors appears equally often (that is, the matrix is orthogonal). A more concise notation of each of the eight runs is shown in the fifth column, consisting of run orders in which only factors in the upper levels are depicted. The final column shows the values of the response variable (y) that result from each run i.

From these set runs, it is feasible to develop a mathematical model that can be used to infer the response from a given combination of factor values. If x's are quantities known for each experimental run, such models with p parameters are generically represented by

$$y = \beta_0 + \sum_{i=1}^{p} \beta_i x_i + \sum_{i=1}^{p-1} \sum_{j=i+1}^{p} \beta_{ij} x_i x_j + \epsilon, \tag{2.1}$$

where the first term is the global mean; the second term represents the main effect of each factor; the third term represents the effects of two-factor interactions; ε is a random error component; and β_i and β_{ij} are the coefficients to be estimated by the least squares method (Alonso et al., 2011).

Literature provides criteria for selecting run orders that take into account the cost of controlled variables (Bhowmik et al., 2017, Hilow, 2013, Wilmut and Zhou, 2011, Street and Burgess, 2008, Tack and Vandebroek, 2004a, Fisher, 1926). Dickinson (1974), Draper and Stoneman (1968) and Daniel and Wilcoxon (1966), for instance, use the *number of factor changes values* (NFC). Although the transition cost may vary for each factor, we assume that the larger the number of the factor changes, the more expensive the design. For a 2^k factorial design with ($n > 1$) runs, it is given by

$$\text{NFC} = \sum_{i=1}^{n-1} \sum_{j=1}^{k} |\mu_{ij} - \mu_{(i+1)j}|, \tag{2.2}$$

where μ_{ij} is the level of factor j in ith experiment that is performed in the run order with $\mu_{ij} \in \{-1, +1\}$. For the 2^3 factorial experiment shown in Figure 1, lexicographic run order $\langle 1\ a\ b\ ab\ c\ ac\ bc\ abc \rangle$ (that is, experiment 1 followed by experiment 2, followed by experiment 3, and so on) has NFC = 11. The minimum NFC value is 7, which can be obtained with run order $\langle a\ ab\ b\ bc\ abc\ ac\ c\ 1 \rangle$.

In addition to cost considerations, one problem that is faced by the investigator while designing experiments is ensuring their robustness, that is, avoiding the influence of linear time trends (Hilow, 2013). Linear time trends arise in the presence of uncontrolled factors and invalidate the premise of independence among the different response variable values (the independence of control variables, on the other hand, is ensured by the orthogonality of design matrices).

Alonso et al. (2011) applied metaheuristic Simulated Annealing to orthogonal fractional-factorial designs to obtain the minimum number of runs that result in uncorrelated main effects for symmetrical and asymmetrical factorials. Bhowmik et al. (2015) proposed a method for obtaining minimally changed run orders in symmetric factorial experiments; the authors developed an exhaustive search procedure for generating all possible minimally changed run orders that are robust to time trends in factorial experiments. For an interesting discussion on the rationale for using 2^k and 2^{k-p} designs that are robust to linear and quadratic trends, the reader is referred to Mee and Romanova (2010). The authors also present an example to demonstrate the analysis of trend-robust designs.

A good, although indirect, measure of trend effects of a given run order is provided by the maximum bias absolute value (MBAV), which is also known as the maximum time count. Proposed by Draper and Stoneman (1968) for the evaluation of linear time trend effects in 2^3, 2^{4-1}, 2^{5-2}, 2^{6-3} and 2^{7-3} factorial experiments with equal variable change costs and extended by Dickinson (1974) for 2^4 and 2^5 factorial experiments, MBAV provides information about the quality of the run order randomization and is also applicable to models with nonlinear time trends. For 2^k factorial design with n runs, it is given by

$$\text{MBAV} = \max_{j\in 1,\dots,k}\left\{\left|\sum_{i=1}^{n}\theta_i \times \mu_{ij}\right|\right\}, \tag{2.3}$$

where θ_i is the order in which experiment i is performed and μ_{ij} is the factor level in experiment i ($\mu_{ij} \in \{-1, +1\}$). For the 2^3 factorial experiments shown in Figure 1, run order $\langle abc\,1\,c\,ab\,b\,ac\,a\,bc\rangle$ has $\max_{j\in 1,\dots,k}\{|0|, |0|, |0|\} = 0$; that is, it provides the minimal maximum absolute bias value. In contrast, the minimal NFC run order, namely, $\langle a\,ab\,b\,bc\,abc\,ac\,c\,a\rangle$, has $\text{MBAV} = \max_{j\in 1,\dots,k}\{|-8|, |-8|, |-8|\} = 8$. As expected, these two criteria may be conflicting for some designs.

To obtain the best trade-off between good statistical properties and low cost, various methods have been proposed (Bhowmik et al., 2015, Correa, Grima, Pere and Tort-Martorell, 2009, Tack and Vandebroek, 2004b, Coster and Cheng, 1988, Steinberg, 1988, Joiner and Campbell, 1976). Draper and Stoneman (1968) and Dickinson (1974) performed a complete enumeration of run orders and suggested selecting the run order based on the analysis of MBAV and NFC values. This procedure is limited to relatively small design matrices, given the computational effort required for the enumeration.

In Wang and Jan (1995), some properties of columns in orthogonal matrices are used to define rules for constructing run orders in order to avoid time effects and reduce costs. Cheng, Martin and Tang (1998) proposed a method for constructing designs with minimum and maximum NFC among all designs of experiments with resolution φ, for $\varphi = III$ and $\varphi = IV$. Tsao and Liu (2008) presented an algorithm that sequences experimental designs for which there are only m non-zero effects/interactions, so that only the first m run orders in the sequence are required for estimating such effects. Jacroux (1994) proposes a technique that constructs trend-resistant fractional designs with two or more factor levels. Other procedures that take into account the trade-off between cost and time-trend effects in experimental design have been reported in Bhowmik et al. (2015), Wang and Chen (1998), and Wang (1991), among others.

Other methods explore efficiency concept to select the array and sequence of runs (Pinto and de Leon, 2014, Alonso et al., 2011, Tack and Vandebroek, 2004a, Atkinson, Donev and Tobias, 2007). The D-efficiency of an experimental design provides information about the quality of coefficient β_j estimators of the model (2.1) and is given by

$$D_{\text{eff}} = \frac{|X'X|^{1/p}}{n}, \tag{2.4}$$

where X is the design matrix, n is number of experimental units, p is the number of parameters in the model, and $|X'X| = \det(X'X)$. Note that the maximization of $\det(X'X)$ minimizes the variance and covariance of minimum square estimators of coefficients β_j (Atkinson, Donev and Tobias, 2007). Therefore, the run order with maximum determinant provides the best estimate of the response variable.

In Angelopoulos, Evangelaras and Koukouvinos (2009), a constructive method is proposed for identifying the most D-efficient design with n runs, q columns, and linear and quadratic trend effects with the minimum number of level changes. Designs are generated so that the main effects are independent of linear and quadratic time trends.

The traditional DoE guidelines defend the random order since it generally leads to low MBAV values. In general, these guidelines state that the nature of the application and the practitioner's experience are essential for deciding whether linear time trends should or should not be considered when selecting and sequencing experimental units. Furthermore, robust estimates against a linear time trend effect (MBVA $= 0$) may be associated with run orders with many factor level changes. According to Tack and Vandebroek (2004a), these trend-free run orders have low practical value, especially when the cost of changes exceeds the budget. The uncertainty of the linear time trend effect and the cost of changing factor levels support the search for budget-constrained run orders, which offer the best protection against a postulated time trend and highly justify the study of the trade-off between NFC and MBAV, particularly in industrial settings.

Finding the optimal experiment sequence according to NFC or MBAV criterion (or both) is a combinatorial problem, which explains why the required computational effort severely limits the size of the problem to be solved. The following sections show that this can be overcome by applying operations research techniques, particularly using mathematical programming models.

3 Optimization of experiment run orders

Experiment Sequencing Problem (ESP) can be described as follows: Given a complete graph $G(V, A)$ with n vertices, ESP consists of obtaining the best path that reaches each vertex v_i ($v_i \in V, |V| = n$) exactly once. Each vertex corresponds to an experiment i and each edge (i, j) represents the change of factor level when experiment i is followed by experiment j. Therefore, a feasible solution consists of a permutation of $\pi(1), \pi(2), \dots, \pi(n)$ vertices, in which $\pi(i)$ represents the ith reached vertex.

ESP is a bi-objective problem in which both the run order (path) cost and its maximum absolute bias value are to be minimized. A ghost experiment was used (indexed by $i = 0$) which defines the beginning and end of any path and transforms it into an Hamiltonian cycle; edges $(i, 0)$ and $(0, i)$ ($i = 1, \dots, n$) are of length zero.

The following notation is used for the description of model:

Parameters

- $n + 1$ number of runs ($i = 0$ indexes the ghost experiment)
- μ_{ij} factor level j in experiment i ($i = 1, \dots, n$; $j = 1, \dots, k$)
- c_{it} transition cost from experiment i to t ($c_{it} = \sum_{j=1}^{k} |\mu_{ij} - \mu_{tj}|, i, t = 1, \dots, n; 0$, otherwise)
- M is a large positive number
- S is a small positive number

Decision variables

$$x_{it} = \begin{cases} 1, & \text{if runs i directly precedes experiment } t \\ 0, & \text{otherwise } (i, t = 0, \ldots, n; i \neq t) \end{cases}$$

y_i auxiliary variables ($y_i \in R^+, i = 1, \ldots, n$)
θ_i order in which experiment i is performed in the run order ($\theta_i \in Z^+, i = 0, \ldots, n$)
Z_1 number of changes to factor values (NFC)
Z_2 maximum absolute bias value (MBAV)

The mono-objective version of the problem can be described by a mixed-integer 0–1 programming model as follows:

$$\text{minimize} \quad Z_1 + S \times Z_2 \quad \text{or} \tag{3.1}$$

$$Z_2 \tag{3.2}$$

$$\text{subject to} \quad \sum_{i=0}^{n} x_{it} = 1, \quad \forall t = 0, \ldots, n, t \neq i \tag{3.3}$$

$$\sum_{t=0}^{n} x_{ij} = 1, \quad \forall i = 0, \ldots, n, i \neq t \tag{3.4}$$

$$y_i - y_t + (n+1) \times x_{it} \leq n, \quad \forall i = 0, \ldots, n, \forall t = 0, \ldots, n, i \neq t \tag{3.5}$$

$$Z_1 = \sum_{i=0}^{n} \sum_{t=0}^{n} c_{it} \times x_{it}, \quad t \neq i \tag{3.6}$$

$$\theta_0 = 0 \tag{3.7}$$

$$\theta_t \geq \theta_i + 1 + M \times (x_{it} - 1), \quad \forall i = 0, \ldots, n, \forall t = 1, \ldots, n, i \neq t \tag{3.8}$$

$$\theta_i \leq n, \quad \forall i = 1, \ldots, n \tag{3.9}$$

$$-Z_2 \leq \sum_{i=1}^{n} \theta_i \times \mu_{it}, \quad \forall t = 1, \ldots, k \tag{3.10}$$

$$Z_2 \geq \sum_{i=1}^{n} \theta_i \times \mu_{it}, \quad \forall t = 1, \ldots, k \tag{3.11}$$

$$x_{it} \in \{0, 1\}, \quad \forall i = 0, \ldots, n \tag{3.12}$$

$$y_i \in R^+, \quad \forall i = 0, \ldots, n \tag{3.13}$$

$$\theta_i \in Z^+, \quad \forall i = 0, \ldots, n \tag{3.14}$$

The objective function (3.1) is used when the aim is to find a run order with minimum NFC. In addition to NFC (which is fully described in equation (3.6), function (3.1) includes a second term for computing MBAV (see the following paragraph). Parameter S is sufficiently small so that Z_1 greatly dominates Z_2. Equations (3.3) and (3.4) respectively, ensure that only one experiment can follow and precede each experiment, inequalities (3.5) eliminate subcycles and constraints (3.12) and (3.13) define the domains of variables x and y, respectively.

Objective function (3.2) is applied when run orders with minimum MBAV are required. The MBAV computation uses constraints (3.7)–(3.11). Specifically, equations (3.7)–(3.9) compute the order θ_i in which each experiment i is performed (in equation (3.7), note that the ghost experiment was performed first), while constraints (3.10)–(3.11) consist of the linearization of $Z_2 = \max_{t \in 1,\ldots,k}\{|\sum_{i=1}^{n} \theta_i \times \mu_{it}|\}$. This set of constraints requires Z_2 to be minimized, which is naturally performed in (3.2). Finally, constraint (3.14) defines the domain of variable θ.

A bi-objective version of the model can be obtained by maintaining either (3.1) or (3.2) as the objective function and using the other objective as a constraint. For example,

$$\begin{aligned} \text{minimize} \quad & (3.1) \\ \text{subject to:} \quad & (3.3)\text{–}(3.14) \\ & Z_2 \le \varepsilon_2, \end{aligned} \tag{3.15}$$

where ε_2 is the maximum acceptable maximum absolute bias value.

Applying an exact method to solve the bi-objective model [(3.1); (3.3)–(3.14)] with appropriate decreasing ε_2 values allows the computation of one feasible solution for each point of the Pareto front, which is the subset $\overline{Z} = (\overline{Z_1}, \overline{Z_2})$ of the objective space associated with all (Pareto) efficient solutions. A feasible solution $\boldsymbol{x}$ is efficient if there is no other feasible solution $\boldsymbol{x}'$ so that $Z_g(\boldsymbol{x}) \le Z_g(\boldsymbol{x}')$ for $g = 1, 2$, with at least one strict inequality. Although finding the Pareto front is usually a time-consuming process, it clearly reveals the trade-off between the minimum cost and the maximum absolute bias value, thereby allowing the decision-maker to choose the preferred solution from the set of generated solutions.

4 Computational experiments

Experiments were performed using microcomputer with Intel Core2 i7 2.67 GHz processor and 12 GB of RAM. Modelling language GAMS 2.3 with CPLEX 11.0 solver was used to solve models. CPLEX 11.0 uses a branch-and-cut method for mixed linear programming models and supports parallel processing (Rosenthal, 2014). Default parameters of CPLEX, null tolerance for the optimality gap, parallel processing (4 threads), and maximum runtime of 36,000 seconds (10 hours) were used for each problem to be solved. Experiments involved two sets of 10 examples each. The examples in Set A consist of orthogonal matrices with 8 to 64 runs and 3 to 6 factors. Set B was first approached in the work of Angelopoulos, Evangelaras and Koukouvinos (2009); examples consist of matrices with 12 to 28 runs and 4 to 6 factors. Non-regular designs provide an alternative to the full factorial and regular fractional factorial designs (Angelopoulos, Evangelaras and Koukouvinos, 2009). For non-regular designs (12, 20, 24 and 28 runs), a statistical package was used to obtain designs with D-optimal using Dykstra DETMAX algorithm to order them.

4.1 Minimizing NFC-Set A

Table 1 presents the results obtained for the 10 examples of Set A with the model [(3.1); (3.3)–(3.14)], that is, with the objective of minimizing NFC. For each example, the second column presents the number of factors of the design of experiments by k and f when there is experiment fractionation, with resulting number of runs (2^{k-f}) and resolution type. The following three columns show, for a given design, the run order that is returned by GAMS/CPLEX and associated NFC and MBAV values. Time column presents the time required to obtain the *first feasible run order with optimal NFC value* and the total runtime (in parentheses); both given in seconds. For each example, the optimal run order value is identified by analysing the lower bound in the GAMS output log at the time the run order is found. Run orders presented in the table do not necessarily correspond to optimal run orders, since MBAV in the objective function (3.1) is usually not able to prove that such solutions are optimal in terms of NFC.

Run orders with minimum NFC were obtained for Examples 1–8. In these cases, the times required to obtain the first optimal run order are very short, usually less than one second. For

Table 1 *Computational results for the mono-objective problem* (*Set A*)

Example	Design	Run Order	NFC	MBAV	Time [s]
1	$2^3 = 8$ Type FULL	ab b bc c (1) ac abc	7	8	< 1 (< 1)
2	$2^{4-1} = 8$ Type IV	abcd bd (1) ac ab ad cd bc	14	4	< 1 (< 1)
3	$2^{5-2} = 8$ Type III	cd de be bc ace abcde abd a	15	16	< 1 (< 1)
4	$2^4 = 16$ Type FULL	abd bd bcd bc c ac a ad d (1) b ab abc abcd acd cd	15	16	< 1 (32)
5	$2^{5-1} = 16$ Type V	a e bde abd acd bcd bce ace cde abcde abc c b abe ade d	30	0	< 1 (323)
6	$2^{6-2} = 16$ Type IV	cef bef bde abd abf acf acd cde abcdef adef df (1) ae abce bc bcdf	31	16	7 (12)
7	$2^5 = 32$ Type FULL	de ade ad abd abcd bcd bcde cde ce bce bc abc ab a ae e (1) b be abe abce ace ac c cd acd acde abcde abde bde bd d	31	0	< 1 (29, 407)
8	$2^{6-1} = 32$ Type VI	abcf acdf cf bcef abef abde be ab ad acde de ce ac cd bcde bdef bd bf bcdf cdef df adef abdf af ae (1) ef acef abcdef abce bc abcd	62	6	< 1 (36,000)
9	$2^{7-2} = 32$ Type IV	abcdf abd abdeg abcdefg cdefg deg d cdf acf a aeg acefg bcefg beg b bcf cg fg ef ce abce abcg abfg abef bdef bcde bcdg bdfg adfg adef acde acdg	63	0	7613 (36,000)
10	$2^{7-1} = 64$ Type V	abdf abfg abeg abde abce abcefh abdefh abefgh efgh eg ce ch gh fg cdfg cf df dh cdgh cdeg de defh cefh cdefgh abcdefgh abcdeg abcdfg abcf abch abdh abcdgh abgh acegh adegh adg adfgh bdfgh bcfgh bcdfh acdfh acd acdeh acdef bcdef bcdeh bcegh bcefg bcg bcd bdg b a aeh beh bef bfh afh acfgh acg acefg aef adefg bdefg bdegh	127	20	33,996 (35,275)

the remaining two examples, the best lower bounds produced by GAMS/CPLEX are close to those of the most feasible solutions; the gaps are smaller than 1.6%, which means that the cost of the optimal solution (in terms of NFC) is one unit lower. For Example 10, GAMS/CPLEX ran out of memory before the maximum allowed runtime had elapsed.

4.2 Minimizing NFC subject to MBAV—Set A

The bi-objective model [(3.1); (3.3)–(3.14); (3.15)] was iteratively solved as described in Bérubé, Gendreau and Potvin (2009), that is, with decreasing ε_2 values, each of which equals to the MBAV value (Z_2), that was found in the previous iteration, decremented by one unit. Initial ε_2 value was obtained by solving model [(3.2); (3.3)–(3.14)] with Z_1 equal to the NFC value obtained with the model [(3.1); (3.3)–(3.14)]. The final ε_2 value was bounded by the MBAV value obtained by solving the model [(3.2); (3.3)–(3.14)]; however, the procedure was halted if no feasible solution was found for a given ε_2 within the available runtime. Non-efficient solutions found during the process were excluded by inspection. Note that since the decision variables in Z_1 and Z_2 functions have integer values, if GAMS/CPLEX succeeds in proving the optimality of solutions for each ε_2 or the infeasibility of the model, the procedure produces one feasible solution for each point of the Pareto front.

Table 2 shows the results obtained. The following three columns present, for a given design, the run orders that result from each iteration, associated NFC value, and associated MBAV value. Time column presents the time required to find the best solution and the total runtime (in parentheses); both given in seconds. Runtimes include solving the models that provide the initial and final ε_2 values and exclude (final) iterations that fail to produce feasible solutions.

Pareto fronts were obtained for Examples 1–5 and 7. In these cases, the runtime per run order is much longer than that required with the mono-objective model, sometimes reaching more than 8 hours. For Examples 6 and 8–10, relative gaps vary from 0.001% to 10.8%. For Example 9, only model [(3.1); (3.3)–(3.14); (3.15)] was solved, given that the resulting MBAV is zero. The run order for Example 10 also corresponds to the best feasible solution obtained by solving model [(3.1); (3.3)–(3.14); (3.15)] since GAMS/CPLEX was unable to provide an integer solution for model [(3.2); (3.3)–(3.14)].

For Examples 2 and 3, the minimum MBAV is greater than zero. This result reveals that it is not always possible to obtain trend-free run orders for any set of experimental units. If we replace runs in Example 2 by [*ab abc acd ad bcd bd c* (1)], the optimal trend-free run order [*bd acd c ab abc* (1) *ad bcd*] with NFC = 17 is obtained in less than 1 second when model [(3.2); (3.3)–(3.15)] is solved. Similar result was obtained for Example 5: run order with NFC = 25 and MBAV = 0 is obtained in 99 seconds. Although the aforementioned designs have maximum efficiency (100%), their resolutions are lower than those presented by matrices adopted in this work.

Figure 2 shows the Pareto fronts found for Examples 1–4. Examples 5 and 7 are omitted since they are the only optimally proven cases for which the two objectives do not conflict, thereby providing a single solution each.

4.3 Minimizing NFC subject to MBAV—Set B

In this section, solutions for the bi-objective model are compared to results reported in Angelopoulos, Evangelaras and Koukouvinos (2009). Their procedure (henceforth referred to as AEK09) constructs sets of linear time trend run orders (MBAV = 0) while considering the trade-off between the matrix D-efficiency values and NFC. In addition to the trade-off analysis between NFC and MBAV, computational experiments allow us to determining whether it is possible to obtain equal or less costly linear time trend run orders from higher-efficiency matrices, which are provided by *Statistica* (Statsoft). The bi-objective model was solved by decreasing the ε_2 values, with final ε_2 value equal to zero, rather than by solving the model [(3.2); (3.3)–(3.14)].

Table 3 presents the results obtained. For each of the 10 examples of Set B, the second column presents the number of runs n and k factors of the design. The next three columns provide, for a given example and for each source (AEK09 or Model), the matrix D-efficiency value (D-Eff), the NFC value, and the MBAV value. Time column presents the time required to reach the best feasible solution and the total CPU time (in parentheses); both given in seconds. Runtimes exclude (final) iterations that fail to produce feasible solutions. The last column lists the run orders obtained by each source. For cases in which Angelopoulos, Evangelaras and Koukouvinos (2009) report alternative run orders, only the first is presented.

Pareto fronts were obtained for Examples 1, 2 and 5. Linear time trend run orders with equal NFC values were obtained for Examples 2 and 5, and 24% smaller NFC was found for

Table 2 *Computational results for the bi-objective problem* (*Set A*)

Example	Design	Run Order	NFC	MBAV	Time [s]
1	$2^3 = 8$ Type FULL	ab b bc c (1) a ac abc	7	8	<1 (<1)
		a b bc c ac abc ab (1)	9	2	<1 (<1)
		c b ab ac a abc bc (1)	11	0	1 (1)
2	$2^{4-1} = 8$ Type IV	abcd bd (1) ac ab ad cd bc	14	4	<1 (<1)
		bd ac bc ad ab cd (1) abcd	22	2	2 (2)
3	$2^{5-2} = 8$ Type III	cd de be bc ace abcde abd a	15	16	<1 (<1)
		a cd bc be de ace abcde abd	16	8	<1 (<1)
		abd cd ace a be de abcde bc	19	6	1 (2)
		abd ace de be bc cd abcde a	20	4	<1 (3)
		abcde a de bc be cd abd ace	24	2	1 (1)
4	$2^4 = 16$ Type FULL	abd bd bcd bc c ac a ad d (1) b ab abc abcd acd cd	15	16	<1 (17)
		cd bcd b ab a ac acd ad abd bd d (1) c bc abc abcd	16	12	325 (399)
		abcd abc c (1) b bd abd ad d cd acd ac a ab bc bcd	17	4	2380 (4260)
		bcd cd (1) b ab a acd abcd abd ad ac abc bc c d bd	19	0	430 (13,550)
5	$2^{5-1} = 16$ Type IV	a e bde abd acd bcd bce ace cde abcde abc c b abe ade d	30	0	167 (167)
6	$2^{6-2} = 16$ Type IV	cef bef bde abd abf acf acd cde abcdef adef df (1) ae abce bc bcdf	31	16	<1 (6)
		adef abcdef abce bc (1) df bcdf abf ae cde cef acf acd abd bde bef	33	12	27 (254)
		acf bef bde cde acd abd abf abcdef cef (1) df adef ae abce bc bcdf	35	8	221 (13,154)
		abf cef cde acd abd bde bef df acf abcdef abce bc (1) ae adef bcdf	37	2	430 (13,550)
7	$2^5 = 32$ Type FULL	de ade ad abd abcd bcd bcde cde ce bce bc abc ab a ae e (1) b be abe abce ace ac c cd acd acde abcde abde bde bd d	31	0	15,237 (15,237)
8	$2^{6-1} = 32$ Type VI	abcf acdf cf bcef abef abde be ab ad acde de ce ac cd bcde bdef bd bf bcdf cdef df adef abdf af ae (1) ef acef abcdef abce bc abcd	62	6	668 (72,000)
9	$2^{7-2} = 32$ Type IV	abcdf abd abdeg abcdefg cdefg deg d cdf acf a aeg acefg bcefg beg b bcf cg fg ef ce abce abcg abfg abef bdef bcde bcdg bdfg adfg adef acde acdg	63	0	3945 (36,000)
10	$2^{7-2} = 32$ Type IV	abdf abfg abeg abde abce abcefh abdefh abefgh efgh eg ce ch gh fg cdfg cf df dh cdgh cdeg de defh cefh cdefgh abcdefgh abcdeg abcdfg abcf abch abdh abcdgh abgh acegh adegh adg adfgh bdfgh bcfgh bcdfh acdfh acd acdeh acdef bcdef bcdeh bcegh bcefg bcg bcd bdg b a aeh beh bef bfh afh acfgh acg acefg aef adefg bdefg bdegh	127	20	33,996 (35,275)

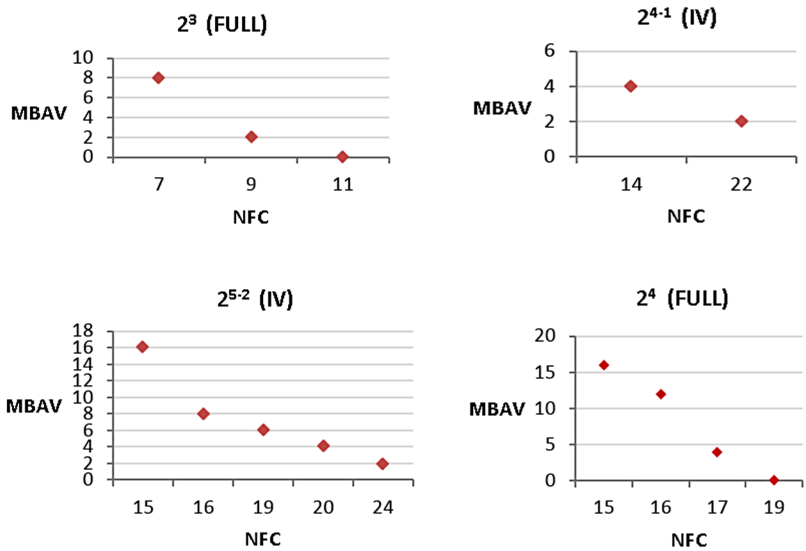

Figure 2 *Pareto fronts for Examples* 1–4 (*set A*).

Example 1. Since all matrices used by the model have equal or higher efficiency compared to those constructed by AEK09, this result indicates that better trade-offs between efficiency and cost are possible. In contrast, higher NFC values were obtained for Examples 4, 7 and 10, which represent 3.5 to 27.8% quality deterioration relative to corresponding solutions provided by AEK09. However, according to the lower-bound analysis, the best possible NFC values in these cases are 30, 46 and 54, respectively, which are larger than those for the corresponding AEK09 solutions. This indicates that the selection of experiments based on the maximization of the matrix efficiency clearly conflicts with the minimization of run order costs. For Examples 3 and 8, the bi-objective model was unable to find an integer solution within the maximum running time when ε_2 (MBAV) was smaller than 2 and 4, respectively. For Examples 6 and 9, gaps relative to the best lower bounds vary from 0.0013% to 16.7%.

4.4 Illustrative example

An Illustrative example where randomization experiment is inadequate is a glass container manufacturing process used in the food industry (Oprime, Pureza and Oliveira, 2017). A brief description of this process indicates four macro-stages:

1. Merging stage, in which the chemical properties of the molten liquid has a significant influence on the quality of the final product;
2. Hot-forming stage, which key elements are mechanical components and operating procedures;
3. Product cooling stage, which final quality depends on the cooling cycle; and finally,
4. Final inspection of 100% products stage, which critical variable is the inspection equipment instability. This stage is a factor that may produce linear trend effects due to the loss of accuracy in the measurement system over time.

Five factors (defined as A, B, C, D, and E) related to the manufacturing process were selected: (i) melting process parameters; (ii) lubrication of melting molds; (iii) features of the raw materials used in the fusion; (iv) shaping process parameters; (v) lifecycle of the equipment used in the shaping stage. The response variable process yield (number of defectless bottles), and is expressed in percentage. This illustrative example, practitioners may be considering

Table 3 *Computational results for the bi-objective problem* (*Set B*)

Example	$n \times k$	Source	D-Eff [%]	NFC	MBAV	Time [s]	Run order
1	12×4	AEK09	81.41	25	0	–	(1) abcd ac ad bcd bd ab bc c d ab acd
		Model	85.78	12	14	0.5 (1)	bc c ac a ad d bd b ab abc abcd cd
				13	10	4 (6)	ab a ac c cd bd b bc abc abcd ad d
				14	6	9 (15)	ab abc ac cd d bd b bc c a ad abcd
				15	4	12 (83)	c ac b bd abcd abc ab a ad d cd bc
				17	2	53 (314)	abc ac a bd b d cd c bc ab abcd ad
				19	0	27 (1024)	cd ab b bc ad a ac c abc abcd bd d
2	16×5	AEK09	100.0	30	0	–	(1) ab abcd abce acde de ce cd bd bcde be ae abde ad ac bc
		Model	100.0	30	0	100.0 (100.0)	c b bde cde ade abe abc acd abcde ace a abd d bcd bce e
3	20×4	AEK09	93.95	19	0	–	(1) (1) bd bcd bcd abc ac acd acd ad a abc abd abd ab b bc c cd d
		Model	96.69	15	14	22 (142)	ad acd cd bcd bc b ab a a ac c c (1) d d bd abd abcd abcd abc
				16	4	1855 (7611)	d ab abc b bcd c a cd abcd ac acd abd (1) ad bcd bd c ad ab abcd d b bc ac
				17	2	18,941 (36,000)	abcd abcd acd d d (1) c c bc abc ab ab b b bd abd ad ad a ac ac cd bcd bcd
4	20×5	AEK09	86.61	29	0	–	(1) ae ab acd acde abcde bce bc bcd bd abde bde e ce cde d ad ac abc abe
		Model	95.14	30	0	2008 (36,000)	bce bce ace a a b b d bde abd abe abe ade acd bcd abcde abc c e cde
5	24×4	AEK09	96.84	17	0	–	(1) (1) a abd abd abcd acd acd cd c bc bc bcd bcd bd b ab ab abc ac ac ad d d
		Model	96.84	15	12	202 (200)	ab ab abc bc c c cd d d ad ad abd bd bcd bcd abcd abcd acd ac ac a (1) b b
				17	0	1879 (13,774)	abcd abcd abd d d (1) b b bc abc ac ac c c cd acd ad ad a ab ab bd bcd bcd

Table 3 (*Continued*)

Example	$n \times$k	Source	D-Eff [%]	NFC	MBAV	Time [s]	Run order
6	24 × 5	AEK09	93.90	30	0	–	(1) (1) ad ade abde abcd abce abce bcde bcd cd bc be be ce cde acde ae ac ac ab abd bd de
		Model	94.28	30	6	4825 (36,000)	b b abc abc ace ace cde e e abe abe a a c c bcd bce bce bde ade d acd abcde abd
				32	0	2320 (36,000)	b b e e abe ace ace abcde abc abc c c acd a a abe bce bce bcd cde d bde abd ade
7	24 × 6	AEK09	79.26	36	0	–	(1) ac acdf abcdf abdef bde bd bf bef cef ce cde abcde abce abcef aef af ad ade def cdf bcdf bc ab
		Model	82.04	46	4	4988 (36,000)	abcf ab (1) ae af bf bc cf cd acdf ad ac abce abcd bd be abef bcef ce acef abcdef abdf df de
8	28 × 4	AEK09	97.12	21	0	–	(1) a ac cd c bc bcd bcd bd bd abd abd ad a ab ab abc abc abcd acd acd acd d d (1) c bc b
		Model	97.94	15	28	9 (197)	ab ab b b (1) c c cd cd acd abcd abcd abd abd bd bd d d ad ad a a ac ac abc bc bc bcd
				16	8	1792 (4707)	ad ad abd abd ab b b bc bc c c ac ac acd cd cd bcd bd bd d d (1) a a ab abc abcd abcd
		Model	97.94	17	6	1536 (36,000)	b b ab a a ad ad abcd abcd acd cd cd bcd bc bc c c (1) d d bd bd abd abd ab abc ac ac
				18	4	4553 (36,000)	d d ad ad ab ab b b bc bc abc abcd abcd bcd cd cd acd a a ac ac c c (1) bd bd abd abd
9	28 × 5	AEK09	94.09	32	0	–	(1) a ac acd acde abde abde bd bd bcde bcde ce ce e be abe abce abc abcd bc bc cd d de ae ab ad acde
		Model	96.10	30	4	1885 (36,000)	a ad abd ab b bc bce ce cde de ade abde abcde abcd abc ac c (1) e ae abe abce ace acd d bde bd bcd
				36	2	10,049 (36,000)	abe ab abd bd bcd cde ac ace ae e (1) d ad a ce bce bc abce abc abcd acd abcde abde ade de bde b c
10	28 × 6	AEK09	88.55	45	0	–	(1) (1) bc bce abcef abcde abcdf bdf df def ef aef abdef abd ad ace ae acd acdef cde cd bcf cf acf abf ab be bde bcdef
		Model	91.67	54	6	24,141 (36,000)	ae ab abcd bc (1) df adef abdf abef abde abce abcf acdf cf cd ce be bf bcef bcde de bd bdef abcdef acef af ac ad

the time trend due to the measurement system; as soon, they have used a systematic run order of experiments.

Considering that the experiments are subjected to linear trends, practitioners have selected design of experiment with 16 treatments and 5 factors (16.5), using the run order of example 5, Table 2 ($2^{5-1} = 16$), type VI, with MBVA = 0, and NFC = 30. The analysis of systematic run order has suggested the advantage: systematic methods can generate low-cost experimental designs and more robust to linear trend effects. Another aspect, when practitioners use a systematic sequence approach subjected linear or non-linear time trend, there is no bias in the model parameters estimations.

5 Conclusions and future steps

In this study, the problem of two-level factorial design experiments as a bi-objective mathematical programming model was formulated to obtain run orders with low cost and good statistical properties. As commonly prescribed in literature, the number of factor changes and maximum absolute bias values were used to measure cost and quality, respectively, of a given run order. The performance of the model was assessed by computational experiments on designs that consisted of up to 64 runs with different resolution levels.

Results have shown that GAMS/CPLEX was able to provide Pareto fronts for 45% of examples in both considered data sets. For the first set, the exact Pareto Front was obtained for 60% of cases. Furthermore, 80% of examples in this set were optimally solved when the mono-objective model for cost minimization was adopted. The computational times required to obtain the optimal or sub-optimal solution varied from less than one second to the adopted maximum runtime (36,000 seconds), thereby revealing the difficulties of GAMS/CPLEX in solving larger examples. However, the best lower bounds obtained in these cases were usually very close to the best feasible solutions. In addition, many refinements to the basic algorithm can be applied to improve convergence. These include using reduced costs to eliminate variables, heuristics to generate good solutions so that nodes can be pruned by bounds, problem preprocessing, and strengthening cuts through lifting.

For cases in which design matrices are not full-factorial, the quality of solutions is bound by the chosen experiments. Since in our experiments, the design matrix is a parameter supplied by an outside source, this may result in solutions dominated by other solutions provided by a different matrix. Therefore, the next step in our agenda is to extend the model to include the selection of experiments from a regular design matrix. Other interesting research lines include the consideration of other objectives, such as maximizing the resulting matrix D-efficiency and the development of heuristics and metaheuristics.

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