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New orders of 2^k factorial designs generated by simulated annealing adapted to optimality criteria

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ABSTRACT. Excessive changes in factor levels can lead to a high cost in practice and hinder the conduction of experiments, in addition to adding a higher computational cost and loss of the orthogonality property, resulting in numerical problems in estimating the parameters of a model. The sequential specification of experimental points, seen as treatments in a 2^k factorial design, results in a high-order bias in some factors, which is caused by the accumulation of −1 or +1 signals. This study aimed to propose new designs generated by the simulated annealing technique, respecting the main A-optimal and D-optimal optimality criteria as random execution orders that minimize the order bias. This approach allowed the generation of 2^4 and 2^5 factorials, which were compared to the designs in standard order. The simulated annealing technique is a viable method to generate optimal designs with the same efficiency as the usual designs to obtain A-optimal and D-optimal designs with new execution orders, which minimize the effect of order bias relative to standard order designs. Regarding efficiency, the generated designs were precise in the variance of model parameter estimates, similar to the original designs.

Keywords: bias; efficiency; designs; precision; simulation.

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Introduction

The planning of factorial designs is based on a proposal of experimental point arrangements, which satisfy two objectives: obtaining greater statistical precision in the response associated with a statistical model and a lower possible cost of operation. In this context, an application of these experiments is the performance evaluation of computational systems, which can be applied in industrial automation.

For this purpose, Oprime, Pureza, and Oliveira (2017) proposed a simulation study of a manufacturing process for glass containers used in the food industry with five considerations, as follows: i) parameters of the melting process, ii) lubrication of the fusion molds, iii) characteristics of the raw materials used in the fusion, iv) parameters of the forming process, and v) life cycle of the equipment used in the forming step. In that experiment, the authors performed extensive computational studies to examine execution orders that would optimize statistical criteria regarding the robustness and specification of linear trends.

According to Adams, Cintas, and Llabres (2005) and Correa, Grima, and Tort-Martoreli (2012), any factor executed at the same level repeatedly in the execution order of a 2^k experiment and, therefore, presents a grouping of signals, may generate wrong estimates when there is a change in the order of execution of the experimental points in the case in which the factors have two levels, represented symbolically by +1 and −1.

However, excessive changes in the factor levels can lead to a high cost in practice and hinder the execution of the experiment, in addition to adding a higher computational cost and loss of the orthogonality property, resulting in numerical problems in the estimation of the parameters of a model.

In this context, random search procedures are viable alternatives, but the algorithms may require considerable computational effort depending on the number of factors. The Dickinson algorithm (Dickinson, 1974) is an example in which the possible successors of each row of the design, understood as an experimental point or treatment to be performed, are introduced from the bottom up, causing a high-order bias.

The issue occurs in designs with a number of treatments higher than 64, i.e., 2^6 designs. The exchanges that occur during the execution of the algorithm cannot produce the best sequences if the design in the standard order starts with a high bias.

Therefore, the use of heuristic methods (Elliot, Eccleston, & Martin, 1999) in factorial experimental problems is in line with computational resources. In this sense, a genetic algorithm was used in the sequencing of production and planning of industrial experiments (Abreu & Prata, 2018) to solve the production sequencing problem in an environment of parallel machines unrelated to sequence-dependent preparation times. The proposed hybrid genetic algorithm was tested in randomly generated instances and the solving of a real problem in the granite industry.

Other procedures used in the search for designs that provide a new order of experimental points consisted of the optimality criteria, obtained by Kiefer (1959), which assist in the search for designs that maximize information from the optimization of characteristics of the estimators of the parameters of a model.

The D-optimal criterion is the most common optimality criterion for the generation of a design (Goos & Jones, 2011), in which the determinant of the covariance matrix of the estimators of the model parameters is minimized. Atkinson, Donev, and Tobias (2007) reported that this criterion only aims to minimize the variances, regardless of the effect on covariances. Thus, the information matrix trace is considered as the measure X^tX^{-1}.

The exchange algorithm, proposed by Fedorov (1972), consisting of a heuristic method that starts from an initial design and, from it, performs exchanges replacing its experimental points with new candidates, is one of the most well-known computational methods in the literature used to construct optimal designs in both criteria. This procedure is repeated through an iterative process until some statistical criterion of interest is met.

Optimizing an experiment is important because the execution of a factorial experiment does not always neutralize the effect of undesirable factors. These factors vary according to the nature of the experiment and may influence the response variable depending on how the experimental process is conducted when they are not neutralized.

Adams et al. (2005) and Correa et al. (2012) mentioned that any factor executed at the same level repeatedly in the order of execution of a 2^k experiment presents a grouping of signals and may generate erroneous estimates. However, excessive changes in the levels of factors can lead to a high cost in practice and hinder the execution of the experiment.

Thus, orders of execution that offer a minimum number of changes in the factor levels and minimize the influence of undesirable factors have been widely sought, as treatments in industrial experiments are usually performed sequentially.

In this context, this study aims to propose a new order of execution of experimental points in 2^k factorial experiments using the simulated annealing technique to preserve the properties of D-optimal (Goos & Jones, 2011) and A-optimal designs (Atkinson et al., 2007; Ryan, 2007), in which the order bias is minimized compared to factorial experiments in the standard order.

Material and methods

Absolute bias of maximum order bias

The main method used in this study is a validation of the new designs by the Maximum Bias Absolute Value (MBAV), as suggested by Adams et al. (2005). For a better understanding of the calculation of this bias, consider a 2^3 design, in which the treatments, represented in the rows of Table 1, are executed sequentially in the standard order (Z).

Table 1. 2^3 design in the standard order, including interactions.

Standard order (Z)	Factors and interactions						
	A	B	C	AB	AC	BC	ABC
1	-1	-1	-1	1	1	1	-1
2	1	-1	-1	-1	-1	1	1
3	-1	1	-1	-1	1	-1	1
4	1	1	-1	1	-1	-1	-1
5	-1	-1	1	1	-1	-1	1
6	1	-1	1	-1	1	-1	-1
7	-1	1	1	-1	-1	1	-1
8	1	1	1	1	1	1	1

MBAV is calculated for each factor and interaction considering the count of +1 and −1 signs. Thus, the experiment classification by the signs of the highest ABC interaction (Table 2) shows that the highest MBAV to be committed is estimated at 4 units, as we have 4+ and 4− signs for this interaction.

Table 2. 2^3 design in the standard order classified by the ABC interaction signals.

Standard order (Z)	Factors and interactions						
	A	B	C	AB	AC	BC	ABC
1	-1	-1	-1	1	1	1	-1
4	1	1	-1	1	-1	-1	-1
6	1	-1	1	-1	1	-1	-1
7	-1	1	1	-1	-1	1	-1
2	1	-1	-1	-1	-1	1	1
3	-1	1	-1	-1	1	-1	1
5	-1	-1	1	1	-1	-1	1
8	1	1	1	1	1	1	1

Simply ordering of the ABC interaction effect signals resulted in new execution orders compared to the order originally described in Table 1. Thus, MBAV was calculated for each main effect and interaction. The sum of the row numbers associated with the positive signs is subtracted from the sum of the rows associated with the negative signs and divided by the maximum bias. The calculation of the order biases for factors A, B, and C and interaction AB is shown as follows, and the other interactions follow the same procedure.

$$MBAV_A = \left[\frac{1}{4}(2+4+6+8) - \frac{1}{4}(1+3+5+7)\right] = 1$$

$$MBAV_A = \left[\frac{1}{4}(2+4+6+8) - \frac{1}{4}(1+3+5+7)\right] = 1$$

$$MBAV_B = \left[\tfrac{1}{4}(3+4+7+8) - \tfrac{1}{4}(1+2+5+6)\right] = 2$$

$$MBAV_C = \left[\tfrac{1}{4}(5+6+7+8) - \tfrac{1}{4}(1+2+3+4)\right] = 4$$

$$MBAV_{AB} = \left[\tfrac{1}{4}(1+4+5+8) - \tfrac{1}{4}(2+3+6+7)\right] = 0$$

Procedure for simulation

In line with the proposed objectives, the implementation of the simulated annealing technique in the generation of D-optimal and A-optimal designs provides less MVAB relative to the sequence of the 2^k factorial experiments for k = 4 and 5. The design in the standard order was defined as the initial design, represented by (IR), and the new design was represented by (RP). The description of the operations involved in this process is as follows:
(a) Initial design input (IR), set in the standard order.
(b) A design is generated in the neighborhood of (IR), called a posteriori design (RP).
(c) The criteria used to generate the A-optimal and D-optimal designs were calculated according to expressions (1)−(2) and (3)−(4) for the (IR) and (RP) designs.

$$AIR=Trace[(XIRZIR)'(XIRZIR)]^{-1} \quad (1)$$

$$DIR=Det[(XIRZIR)'(XIRZIR)]^{-1} \quad (2)$$

$$ARP=Trace[(XRPZRP)'(XRPZRP)]^{-1} \quad (3)$$

$$DRP=Det[(XRPZRP)'(XRPZRP)]^{-1} \quad (4)$$

In all criteria, X_{IR} and X_{RP} correspond, respectively, to the matrices of the initial design (IR) given in the standard order and the design generated in the neighborhood of (RP). Z_{IR} and Z_{RP} indicate the vectors with the order of execution of the experimental points of the aforementioned designs.

(d) The decision rule applies:

For the A-optimal design, the design proposed by the algorithm is accepted if $A_{RP} < A_{IR}$. Otherwise, the Boltzmann factor, defined by (5), is calculated when $A_{RP} > A_{IR}$.

$$F_A = exp\left\{-\left(\frac{(Trace(RP)-Trace(IR))}{T}\right)\right\} \quad (5)$$

T indicates the temperature function given by T = (1-step)^c, where c is the cooling constant and step is the step size for cooling, fixed at 0.5.

The same applies to the D-optimal design, in which the design proposed by the algorithm (RP) is accepted in comparison to the determinants if Det (RP) < Det (IR). The Boltzmann factor (6) is used otherwise.

$$F_D = exp\left\{-\left(\frac{(Det(RP)-Det(IR))}{T}\right)\right\} \quad (6)$$

The Boltzmann factors (5) and (6) allowed the acceptance of the new design proposed by the simulated annealing algorithm, conditioned to a random value, generated by the uniform distribution (0.1), represented by U.

The condition U < FA is imposed so that the new network (RP) is accepted as the initial network (IR) when considering the A-optimal design as a reference, and again the process begins until reaching convergence and fixing the number of iterations, n = 10,000.

Similarly, assuming the D-optimal design as a reference, the imposed condition is that U < FD. The execution of this algorithm was performed under these conditions, and MVAB, as well as the efficiencies specified in (7) for the D-optimal design and (8) for the A-optimal design, was calculated with the generated designs (Rady, Abd El-Monsef, & Seyam, 2009).

$$Ef_D = \left(\frac{det(\mathrm{IR})}{det(\mathrm{RP})}\right)^{\frac{1}{p}} \quad (7)$$

$$Ef_A = \left(\frac{Trace(\mathrm{IR})^{-1}}{Trace(\mathrm{RP})^{-1}}\right) \quad (8)$$

Results and discussion

Introducing the designs in the initial standard order, i.e., RI, is necessary to identify the new execution orders of the 2^4 and 2^5 factorial experiments. Table 3 shows the description of the experimental points, in which the first block is limited by the experimental points Z = 1-16, which refer to the 2^4 design, and the continuity of the other points, with the specification of Z = 1–32, including the 5th factor E, complement the 2^5 design.

Table 3. 2^4 and 2^5 factorial designs with the Z standard order.

Z	A	B	C	D	E
1	-1	-1	-1	-1	-1
2	1	-1	-1	-1	-1
3	-1	1	-1	-1	-1
4	1	1	-1	-1	-1
5	-1	-1	1	-1	-1
6	1	-1	1	-1	-1
7	-1	1	1	-1	-1
8	1	1	1	-1	-1
9	-1	-1	-1	1	-1
10	1	-1	-1	1	-1
11	-1	1	-1	1	-1
12	1	1	-1	1	-1
13	-1	-1	1	1	-1
14	1	-1	1	1	-1
15	-1	1	1	1	-1
16	1	1	1	1	-1
17	-1	-1	-1	-1	1
18	1	-1	-1	-1	1
19	-1	1	-1	-1	1
20	1	1	-1	-1	1
21	-1	-1	1	-1	1
22	1	-1	1	-1	1
23	-1	1	1	-1	1
24	1	1	1	-1	1
25	-1	-1	-1	1	1
26	1	-1	-1	1	1
27	-1	1	-1	1	1
28	1	1	-1	1	1
29	-1	-1	1	1	1
30	1	-1	1	1	1
31	-1	1	1	1	1
32	1	1	1	1	1

Given the input of these designs, the results in Figures 1 and 2 show that the simulated annealing technique had a convergence, resulting in the A-optimal and D-optimal designs, following the specifications regarding the step size and the number of interactions. This convergence indicated that the energy variation was minimal, reaching a stable configuration to generate more "balanced" designs that mitigated the agglomeration of +1 or −1 signals.

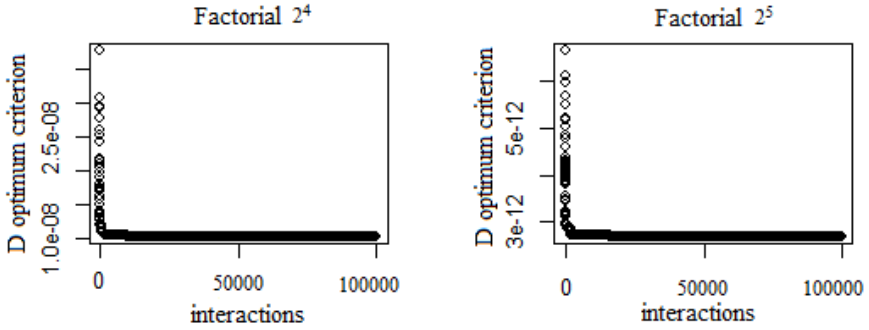

Figure 1. Convergence of the *simulated annealing* algorithm for the designs generated by the D-optimal criterion from the Standard Order.

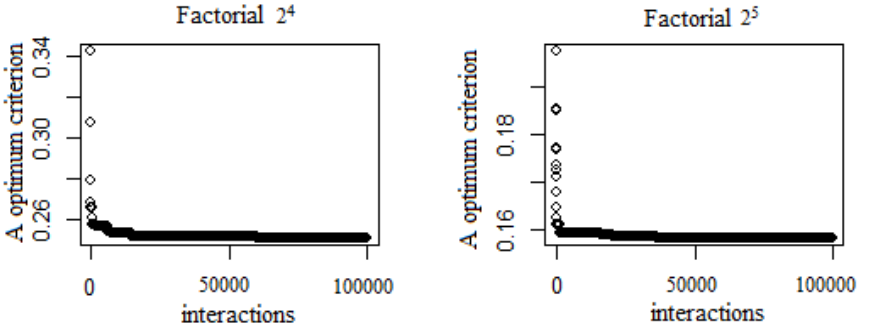

Figure 2. Convergence of the *simulated annealing* algorithm for the designs generated by the A-optimal criterion from the Standard Order.

Table 4 shows the MBAV estimates using as a reference the comparison of the MBAV obtained in the standard order designs, as shown in Table 3.

Table 4. Maximum bias absolute value (MBAV) for the designs obtained by the simulated annealing algorithm (SA).

Design	Factors				
	A	B	C	D	E
2^5 OP	1	2	4	8	16
2^5 A_{SA}	0.188	2.031	4	2.070	3.556
2^5 D_{AS}	0.062	8	3.174	3.556	1.568
2^4 OP	1	2	4	8	-
2^4 A_{SA}	2.158	2.158	3.174	1.396	-
2^4 DAS	0	1	0	0,5	-

Table 4 shows that the A-optimal and D-optimal designs generated for 2^5 had MBAV estimates for all factors compared to the standard order design. The order biases were considered relatively low with a reduction in the number of factors, i.e., 2^4, the A-optimal (A_{SA}) design, except for factor A. This fact did not occur in the comparison of biases related to the design generated with the D-optimal criterion. Therefore, we proceeded with the recommendation of the factorial experiments A-optimal and D-optimal, 2^4 and 2^5, generated by the simulated annealing technique, with the execution orders described in Tables 5 and 6.

Importantly, some experimental points were repeated in both the A-optimal and D-optimal criteria in the execution orders (Tables 5 and 6). The occurrence of this result is advantageous in situations in which the repetition of all experimental points becomes unfeasible either by time or cost of operation. Thus, the necessary information is available with the repetition of some experimental points to estimate the pure error as an alternative to the experimental error, allowing us to make a statistical inference regarding the study of the significance of model parameters. Table 7 shows the results regarding the efficiency of the generated designs.

Table 5. New order of execution for the A-optimal and D-optimal designs obtained by the simulated annealing algorithm for the 2^4 design from the design given in the standard order Z (Table 3).

A-optimal		D-optimal	
$4^{(1)}$	$11^{(9)}$	$14^{(1)}$	$4^{(9)}$
$2^{(2)}$	$16^{(10)}$	$9^{(2)}$	$6^{(10)}$
$14^{(3)}$	$13^{(11)}$	$8^{(3)}$	$15^{(11)}$
$9^{(4)}$	$5^{(12)}$	$4^{(4)}$	$12^{(12)}$
$1^{(5)}$	$11^{(13)}$	$15^{(5)}$	$10^{(13)}$
$16^{(6)}$	$7^{(14)}$	$11^{(6)}$	$7^{(14)}$
$10^{(7)}$	$4^{(15)}$	$1^{(7)}$	$1^{(15)}$
$10^{(8)}$	$6^{(16)}$	$5^{(8)}$	$14^{(16)}$

() sequence of the experimental point to be executed.

Table 6. New order of execution for the A-optimal design obtained by the simulated annealing algorithm for the 2^5 design from the design given in the standard order Z (Table 3).

A-optimal				D-optimal			
$8^{(1)}$	$3^{(9)}$	$8^{(17)}$	$17^{(25)}$	$24^{(1)}$	$3^{(9)}$	$8^{(17)}$	$3^{(25)}$
$32^{(2)}$	$12^{(10)}$	$2^{(18)}$	$21^{(26)}$	$32^{(2)}$	$21^{(10)}$	$24^{(18)}$	$17^{(26)}$
$13^{(3)}$	$7^{(11)}$	$30^{(19)}$	$20^{(27)}$	$31^{(3)}$	$28^{(11)}$	$5^{(19)}$	$17^{(27)}$
$14^{(4)}$	$23^{(12)}$	$9^{(20)}$	$5^{(28)}$	$20^{(4)}$	$12^{(12)}$	$19^{(20)}$	$26^{(28)}$
$9^{(5)}$	$8^{(13)}$	$31^{(21)}$	$16^{(29)}$	$13^{(5)}$	$14^{(13)}$	$32^{(21)}$	$30^{(29)}$
$27^{(6)}$	$11^{(14)}$	$25^{(22)}$	$27^{(30)}$	$15^{(6)}$	$12^{(14)}$	$23^{(22)}$	$6^{(30)}$
$18^{(7)}$	$5^{(15)}$	$30^{(23)}$	$20^{(31)}$	$15^{(7)}$	$31^{(15)}$	$29^{(23)}$	$8^{(31)}$
$31^{(8)}$	$12^{(16)}$	$3^{(24)}$	$10^{(32)}$	$27^{(8)}$	$10^{(16)}$	$11^{(24)}$	$9^{(32)}$

() sequence of the experimental point to be executed.

Regarding the efficiency of the optimal designs generated by the simulated annealing method compared to standard designs, the results showed that the designs had efficiencies similar to the standard design for both criteria (Table 7).

According to Khinkis, Laurence, Faessel, and Greco (2003), the interpretation of the efficiency of a design, for example, D-optimal, is given as a factor, whereby a given design must be replicated to obtain precision of the parameter estimates equal to that of the obtained D-optimal design.

In this context, Khinkis et al. (2003) exemplifies a D-optimal design with an efficiency equal to 0.5, which means that the initial design, from which the D-optimal design was obtained, needs to be replicated twice to achieve the same precision of the D-optimal. Similarly, it follows the interpretation given the specification of the A-optimal criterion.

Table 7 shows the specification of the expression (8), used to calculate the efficiency, referring to the A-optimal criterion, in which the numerator corresponds to the matrix trace (RP), that is, generated by the simulated annealing technique, and the denominator corresponds to the matrix trace with the standard order, i.e. (IR).

An efficiency estimation close to 1 indicates proximity in the variances of the estimates of both designs. This statement is also valid for the D-optimal criterion. Therefore, there is statistical evidence that, in both criteria, the designs with the new orders do not differ in efficiency compared to the original designs regarding the precision of the variances of estimates in the presence or absence of covariance.

Table 7. Efficiency of the main A-optimal and D-optimal designs obtained by the simulated annealing (SA) algorithm.

	Criterion	
Design	A_{SA}	DAS
2^4	0.9320	0.9504
2^5	0.9532	0.9602

Conclusion

The simulated annealing technique is a promising alternative method for the generation of A-optimal and D-optimal designs with new orders of execution that minimize the effect of order bias relative to standard order designs. Regarding efficiency, the generated designs were precise in the variance of the estimates of model parameters, similar to the original designs. Both the new order matrices and the A-optimal and D-optimal matrices obtained from the new order matrices reasonably stabilized the variance of the estimates of factor effects.

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