Multidimensional blocking of Experimental Designs

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Abstract

Fisher's three R's or three principles of designs of experiments are (i) Randomization; (ii) Replications; and (iii) Local control or blocking (also called noise reduction). Of the three, blocking is the most difficult. Works on blocked designs (e.g. blocked fractional factorial designs, blocked response surface designs, etc.) are very limited. In addition, there might be more than one extraneous variations or blocking factors. As such, there is a need for a general method to do multidimensional blocking of experimental designs. This paper extends the idea of orthogonal blocking of Box & Hunter (1957) from one blocking factor to several blocking factors. It then presents an algorithm which can impose several blocking/noise factors on popular experimental designs, including a newer class of designs namely definitive screening designs

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(DSDs) and DSD-based mixed-level screening designs.

Keywords: Box-Behnken designs; Central composite designs; Definitive screening designs; Fractional factorial designs; Orthogonal blocking.

1 Introduction

An experiment is conducted to determine the relationship between input factors affecting a process and the output of that process. There are controllable input factors to be studied as well as uncontrollable ones to be eliminated. While the former can be modified to optimize the output, this is not the case of the latter. Examples of uncontrollable factors are: (i) different batches of raw material; (ii) different machine; (iii) different operators; (iv) different locations; (v) different times, etc. A well-designed experiment minimizes the effects of these uncontrollable factors by partitioning the set of experimental runs into more homogeneous subsets. This noise reduction exercise is called local control or blocking. It makes experiments more sensitive in detecting significant effects and hence less experimentation may be required. Examples of the scenarios when designs of more than one blocking factors can be used are:

Example 1: A 2^5 factorial experiment to identify interaction effects for different additives in linear low-density polyethylene film (Hoang et al., 2004, Mee, 2009, p. 79). The factors and levels are: (**A**) Antioxidant A (ppm), 0 and 400; (**B**) Antioxidant B (ppm), 0 and 400; (**C**) Acid Scavenger (ppm), 0 and 1000; (**D**) Anti-block agent (ppm), 0 and 2000; (**E**) Slip additive (ppm), 0 and 800. As the full 2^5 factorial would take at least three days to complete, it was divided into four blocks. Let's assume the experimenter wishes to add to the model an additional block factor, i.e. times of the day (8AM and 2PM).

Example 2: An experiment to study the response of Nitrogen (**N**), Phosphorus (**P**) and Potash (**K**) when combined with seed rate (**S**) on a variety of rice. The design is two replications of the Box-Behnken design (BBD) for four factors: N, P and K are at 0, 35 and 70 kg/ha and S is at 45, 90 and 135 kg/ha. Since the soil is heterogeneous in both directions, the experimenter wishes to divide the runs of the 4-factor BBD into two rows and three columns. Note that the original 4-factor BBD in 27-runs is only available in three blocks.

Example 3: A 9-factor DSD in 21 runs to investigate the oxidation reactions in homogeneous Co^{2+}/PMS system (Zhang et al., 2018). Its main objective is to evaluate the suitability of the DSD approach in optimizing the operating parameters of Co^{2+}/PMS system and to identify the significant effects involved in the reaction system. See Jones & Nachtsheim (2011) for the use of DSD as a screening design. The nine factors in this experiment are: (1) NaCl, (2) NaH_2PO_4, (3) $NaHCO_3$, (4) $NaNO_3$, (5) Na_2SO_4, (6) HA, (7) PMS, (8) AO II, and (9) Co^{2+}. The first five factors were set at 0, 10, and 20mM, HA at 0, 20, 40mg dm^{-3}, PMS at 2, 6, 10mM. AO II at 50, 75, 100 mg dm^{-3} and Co^{2+} at 0, 0.68, and 1.36mM. Zhang et al. (2018) stated that they could not use response surface designs (RSDs), such as the BBD, the Doehlert design and the central composite design (CCD), as they could not afford the enormous number of runs required by these designs. At the same time, the popular Plackett–Burman design is unable to capture the quadratic and interaction effects. Let's assume the experiment was performed in two different reactors and two different days and the experimenters wish to add these two blocking factors to the model.

2 Conditions for orthogonal blocks

Consider the following model for an n-run design with m factors $x_1, \ldots, x_m$ arranged in b blocks:

$$y_u = \delta_1 z_{1u} + \ldots + \delta_b z_{bu} + \beta_0 + \sum_{i=1}^{m} \beta_{ii} x_{iu}^2 + \sum_{i=1}^{m} \beta_i x_{iu} + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij} x_{iu} x_{ju} + \epsilon_u \tag{1}$$

where y_u $(u = 1, \ldots, n)$ is the response value of the uth run, z_{wu} $(w = 1, \ldots, b)$ the value of the dummy variable, which takes value 1 if the uth run is in wth block and zero otherwise, ϵ_u a random error associated with the uth run. Let $\tilde{z}_{wu} = z_{wu} - \bar{z}_w$, where $\bar{z}_w$ is the mean of $z_{w1}, \ldots, z_{wn}$. Then Equation (1) can be written as:

$$y_u = \delta_1 \tilde{z}_{1u} + \ldots + \delta_b \tilde{z}_{bu} + \tilde{\beta}_0 + \sum_{i=1}^{m} \beta_{ii} x_{iu}^2 + \sum_{i=1}^{m} \beta_i x_{iu} + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij} x_{iu} x_{ju} + \epsilon_u \tag{2}$$

where $\tilde{\beta}_0 = \beta_0 + \delta_1 \bar{z}_1 \ldots + \delta_b \bar{z}_b$ (see Box & Hunter 1957, Section 8 and Khuri & Cornell, 1996, Chapter 8). Equation (2) can now be written in matrix form as:

$$\mathbf{y} = \tilde{\mathbf{Z}}\boldsymbol{\delta} + \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \tag{3}$$

where $\mathbf{y}$ is an $n \times 1$ response vector, $\tilde{\mathbf{Z}}$ a matrix of size $n \times b$ containing b $\tilde{z}_w$ columns in Equation (2), $\boldsymbol{\delta}$ a $b \times 1$ column vector representing block effects, $\mathbf{X}$ is the expanded design matrix of size $n \times p$, $\boldsymbol{\beta}$ a $p \times 1$ column vector of parameters to be estimated, and $\boldsymbol{\epsilon}$ an $n \times 1$ column vector of random errors.

The condition for orthogonal blocks can be written as:

$$\mathbf{X}'\tilde{\mathbf{Z}} = \mathbf{0}. \tag{4}$$

As the sum of the values of the $\tilde{z}$ variables for each run in Equation (2) is zero, i.e. $\sum_{w=1}^{b} \tilde{z}_{wu} = 0$, which is an example of perfect multicollinearity, to avoid the singular data matrix, we replace $\tilde{z}_{bu}$ in Equation (2) by $-(\tilde{z}_{1u} + \ldots + \tilde{z}_{(b-1)u})$. This equation becomes:

$$y_u = \tilde{\delta}_1 \tilde{z}_{1u} + \ldots + \tilde{\delta}_{(b-1)} \tilde{z}_{(b-1)u} + \tilde{\beta}_0 + \sum_{i=1}^{m} \beta_{ii} x_{iu}^2 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij} x_i x_j + \epsilon_u \tag{5}$$

where $\tilde{\delta}_w = \delta_w - \delta_b$ $(w = 1, \ldots, b-1)$. This reparameterization results in dropping the last column of $\tilde{\mathbf{Z}}$ and the last element of $\boldsymbol{\delta}$ in Equation (3). The least square solution for the unknown parameters $\boldsymbol{\delta}$ and $\boldsymbol{\beta}$ in (3) is the solution of the following equation:

$$\begin{pmatrix} \tilde{\mathbf{Z}}' \\ \mathbf{X}' \end{pmatrix} \mathbf{y} = \begin{pmatrix} \tilde{\mathbf{Z}}'\tilde{\mathbf{Z}} & \tilde{\mathbf{Z}}'\mathbf{X} \\ \mathbf{X}'\tilde{\mathbf{Z}} & \mathbf{X}'\mathbf{X} \end{pmatrix} \begin{pmatrix} \hat{\boldsymbol{\delta}} \\ \hat{\boldsymbol{\beta}} \end{pmatrix} \tag{6}$$

When the orthogonal block condition in Equation (4) is satisfied, it can be seen that the solution for $\boldsymbol{\beta}$ from Equation (5) will be the same as the one from the equation $\mathbf{X}'\mathbf{y} = \mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}}$, i.e. the equation for a model without blocking. In other words, for orthogonal block designs, the inclusion of blocks has no effect in the estimation of $\boldsymbol{\beta}$ in Equation (3).

Remarks

1. When there are r blocking factors, the matrix $\tilde{\mathbf{Z}}$ in Equation (3) can be partitioned as $(\tilde{\mathbf{Z}}_1 \ldots \tilde{\mathbf{Z}}_r)$, where $\tilde{\mathbf{Z}}_l$ $(l = 1, \ldots, r)$ is matrix of size $n \times (b_l - 1)$ and b_l the settings of the blocking factor l.

2. Let $\mathbf{x}_i'$ and $\mathbf{x}_u'$ be two rows of $\mathbf{X}$. Let $\tilde{\mathbf{z}}_i'$ and $\tilde{\mathbf{z}}_u'$ be the corresponding vectors of $\tilde{\mathbf{Z}}$. Swapping the ith and uth row of $\mathbf{X}$ is the same as adding the following matrix to $\tilde{\mathbf{Z}}'\mathbf{X}$:

$$-(\tilde{\mathbf{z}}_i - \tilde{\mathbf{z}}_u)(\mathbf{x}_i - \mathbf{x}_u)'. \tag{7}$$

We use this matrix result to develop an algorithm for blocking various types of experimental designs, including DSDs and DSD-based mixed-level designs.

3 Two steps of our blocking algorithm

Here are two steps of our blocking algorithm with r blocking factors using the results in Equation (7):

1. Allocate the n runs of the unblocked design to the blocking factors randomly. Calculate f, the sum of squares of the elements of $\tilde{\mathbf{Z}}'\mathbf{X}$.

2. Repeat searching for a pair of runs such that the swap of the run positions results in the biggest reduction in f. If the search is successful, swap their positions, update f and $\tilde{\mathbf{Z}}'\mathbf{X}$. This step is repeated until f=0 or until f cannot be reduced further.

Remarks:

1. Each computer try has these two steps. Several tries are required for each design and the one with the smallest f will be chosen. For designs with the same f, the one with

the smallest block factor (BF) will be chosen where BF is calculated as:

$$BF = (|X'X|/(|\tilde{\mathbf{Z}}'\tilde{\mathbf{Z}}||\mathbf{X}'\mathbf{X}|))^{1/(p-v)} \quad (8)$$

Here $X = (\mathbf{Z}\ \mathbf{X})$ and $v = \sum_{l=1}^{r}(b_l - 1)$ is the degree of freedom associated with the r blocking factors. Clearly, BF equals 1 means the design is orthogonally blocked.

2. For a response surface design, the orthogonality between the quadratic effects (and main effects) and block variables are considered more important than the orthogonality between 2-factor interactions (2fi's) and block variables. For a factorial or fractional factorial, the orthogonality between main effects and block variables is considered more important than the orthogonality between 2fi's and block variables. For a screening design such as DSD, the orthogonality between main effects and block variables is considered more important than the orthogonality between quadratic effects and block variables. In these situations, partition $\mathbf{X}$ as $(\mathbf{X}_1\ \mathbf{X}_2)$ where $\mathbf{X}_1$ is associated with the more important effects. Partition $\tilde{\mathbf{Z}}'\mathbf{X}$ as $(\tilde{\mathbf{Z}}'\mathbf{X}_1\ \tilde{\mathbf{Z}}'\mathbf{X}_2)$. Let g be the sum of squares of the elements of $\tilde{\mathbf{Z}}'\mathbf{X}_1$ and f the sum of squares of the elements of $\tilde{\mathbf{Z}}'\mathbf{X}$ as defined previously. Step 2 of the algorithm now is: repeat searching for a pair of runs in different blocks such that swapping their run positions results in the biggest reduction in g (or f if g cannot be reduced further). If the search is successful, swap their positions, update f and $\tilde{\mathbf{Z}}'\mathbf{X}$. This step is repeated until f=0 or until f cannot be reduced further.

3. In a sense, our blocking algorithm is an extension of one of Nguyen (2001), which only works with one blocking factors, to several blocking factors. Our blocking algorithm is more general than the one of Gilmour & Trinca (2003), which only work with two blocking

Day	Time	A	B	C	D	E	Day	Time	A	B	C	D	E
1	1	-1	-1	1	1	1	1	2	-1	-1	-1	-1	-1
1	1	-1	1	-1	1	-1	1	2	-1	1	1	-1	1
1	1	1	1	-1	1	1	1	2	1	-1	-1	-1	1
1	1	1	1	1	-1	-1	1	2	1	-1	1	1	-1
2	1	-1	-1	-1	1	-1	2	2	-1	1	-1	-1	-1
2	1	-1	-1	1	-1	1	2	2	-1	1	1	1	1
2	1	1	-1	1	-1	-1	2	2	1	-1	-1	1	1
2	1	1	1	-1	-1	1	2	2	1	1	1	1	-1
3	1	-1	1	-1	-1	1	3	2	-1	-1	-1	1	1
3	1	-1	1	1	-1	-1	3	2	-1	-1	1	1	-1
3	1	1	-1	-1	-1	-1	3	2	1	-1	1	-1	1
3	1	1	1	1	1	1	3	2	1	1	-1	1	-1
4	1	-1	-1	-1	-1	1	4	2	-1	-1	1	-1	-1
4	1	-1	1	1	1	-1	4	2	-1	1	-1	1	1
4	1	1	-1	-1	1	-1	4	2	1	1	-1	-1	-1
4	1	1	-1	1	1	1	4	2	1	1	1	-1	1

Figure 1: A 2^5 factorial with two blocking factors: day and time of the day. The low and high levels are coded as -1 and 1.

factors. Clearly, ours does not require matrix inversions and therefore is considered faster than the ones by other authors (See e.g. Cook & Nachtsheim (1989) and Gilmour & Trinca (2003)).

4 Discussion

In the followings, we will show the solutions for the designs problems mentioned in the Introduction.

Example 1: Figure 1 shows how a 2^5 factorial can be blocked using two blocking factors (day and time of the day) and the model which includes the main-effect and 2fi's terms. Our constructed design is an orthogonally blocked one, meaning the factors **A**, **B**, **C**, **D** and **E** are orthogonal to both days times of day (8AM and 2PM).

Example 2: Figure 2 shows the layout of a replication of the 4-factor BBD, each in two rows and three columns, using the second-order response surface model which include the quadratic terms, the main-effect terms as well as the 2fi's terms. Note that the three center runs have been added to the original 27-run BBD. Like the design in Example 1, the one in this example is an orthogonally blocked one. For both designs, the z-variables associated with the blocking factors have zero correlation with all x-variables in the model.

For the second-order response surface model, the condition for orthogonal blocks (i.e. condition in Equation (3)) is equivalent to the following two conditions (See Box & Hunter, 1957, p. 229):

(i) All sums of x_i's and sum of products between $x_1,\ x_2,\ldots,x_m$ must be zero for each block:

$$\sum_{u}^{n_w} x_{iu} = 0 \text{ and } \sum_{u}^{n_w} x_{iu}x_{ju} = 0,\ (i \neq j,\ w = 1,2,\ldots,b) \tag{9}$$

where the summations include only entries in the wth block.

(ii) For each x_i, $(i = 1,\ldots,m)$, the sum of squares contribution from each block is proportional to the size of the block:

$$\frac{\sum_u^{n_1} x_{iu}^2}{n_1} = \frac{\sum_u^{n_2} x_{iu}^2}{n_2} = \cdots = \frac{\sum_u^{n_b} x_{iu}^2}{n_b}. \tag{10}$$

It can be easily seen that the design in Figure 2 satisfies both conditions in Equations (9) and (10).

Row	Col.	N	P	K	S
1	1	-1	0	-1	0
1	1	-1	0	1	0
1	1	0	0	0	0
1	1	0	1	0	-1
1	1	0	1	0	1
2	1	0	-1	0	-1
2	1	0	-1	0	1
2	1	0	0	0	0
2	1	1	0	-1	0
2	1	1	0	1	0

Row	Col.	N	P	K	S
1	2	-1	0	0	-1
1	2	0	-1	1	0
1	2	0	0	-1	1
1	2	1	-1	0	0
1	2	1	1	0	0
2	2	-1	0	0	1
2	2	0	0	-1	-1
2	2	0	0	0	0
2	2	0	0	0	0
2	2	0	1	1	0

Row	Col.	N	P	K	S
1	3	0	-1	-1	0
1	3	0	0	0	0
1	3	0	0	0	0
1	3	0	0	1	1
1	3	1	0	0	-1
2	3	-1	-1	0	0
2	3	-1	1	0	0
2	3	0	0	1	-1
2	3	0	1	-1	0
2	3	1	0	0	1

Figure 2: One replication of a 4-factor BBD each in two rows and three columns. The low, mid- and high levels are coded as −1, 0 and 1.

Day	Reactor	NaCl	NaH2PO4	NaHCO3	NaNO3	Na2SO4	HA	PMS	AO II	Co2
1	1	-1	0	1	1	1	1	-1	-1	-1
1	1	-1	1	-1	-1	0	1	1	-1	1
1	1	-1	1	0	1	-1	-1	1	1	-1
1	1	0	-1	-1	-1	-1	-1	-1	-1	-1
1	1	0	0	0	0	0	0	0	0	0
1	1	1	-1	1	1	-1	0	1	-1	1
2	1	-1	1	-1	-1	1	0	-1	1	-1
2	1	0	0	0	0	0	0	0	0	0
2	1	0	1	1	1	1	1	1	1	1
2	1	1	-1	0	-1	1	1	-1	-1	1
2	1	1	-1	1	1	0	-1	-1	1	-1
2	1	1	0	-1	-1	-1	-1	1	1	1

Day	Reactor	NaCl	NaH2PO4	NaHCO3	NaNO3	Na2SO4	HA	PMS	AO II	Co2
1	2	-1	-1	-1	1	-1	1	-1	1	1
1	2	-1	-1	1	-1	1	-1	0	1	1
1	2	1	-1	-1	0	1	1	1	1	-1
1	2	1	1	-1	1	1	-1	-1	0	1
1	2	1	1	1	-1	-1	1	-1	1	0
1	2	1	1	1	-1	1	-1	1	-1	-1
2	2	-1	-1	-1	1	1	-1	1	-1	0
2	2	-1	-1	1	-1	-1	1	1	0	-1
2	2	-1	1	1	0	-1	-1	-1	-1	1
2	2	0	0	0	0	0	0	0	0	0
2	2	0	0	0	0	0	0	0	0	0
2	2	1	1	-1	1	-1	1	0	-1	-1

Figure 3: A 9-factor DSD arranged in two rows and two columns. The low, mid- and high levels are coded as −1, 0 and 1.

Example 3: Figure 3 shows the layout of a 9-factor DSD arranged in two rows (reactors) and two columns (days), using the pure quadratic model which includes only the quadratic terms and main-effects terms. Three center runs have been added to the original 21-run DSD. For this design the main effects are clear of block effects but the quadratic effects are partially confounded with block effects. In other words, for this design, unlike the x-variables associated with the main effects in the model, the ones associated with the quadratic effects are not orthogonal to the block effects. It can be seen that the design in Figure 3 satisfies the condition in Equation (9), but not the conditions in Equation (10).

Jones & Nachtsheim (2016) suggested an algorithm to arrange the experimental runs into blocks with well-defined size and provided a real application in the laser etch experiment where the 15-run DSD for four quantitative factors can be divided into three blocks of size five. They pointed out that there were two special situations in which we can very easily construct blocked DSDs: (i) the runs in foldover-pair appearing in a block. A DSD for m factors will thus have m blocks, each containing a foldover-pair; and (ii) the DSD contains two blocks with half of the foldover-pair in each block.

In general, due to the structure of DSDs, it is not possible to use our blocking algorithm to arrange them into orthogonal blocks. To construct orthogonally blocked DSDs, we follow the approach Box & Hunter (1957) for blocking the CCDs. First, we use our blocking algorithm to block the designs into b blocks, making sure that x-variables associated with the main effects are orthogonal to block effects, i.e. Equation (9) is satisfied. We then convert the ± 1 of one or more blocks to $\pm\alpha$ and the calculate α so that Equation (10) is satisfied. Figure 4 shows the 4-factor DSD used for the laser etch experiment (Jones

Block	x1	x2	x3	x4
1	-1	-1	1	1
1	-1	1	-1	0
1	0	-1	-1	-1
1	1	0	1	-1
1	1	1	0	1
2	-1	-1	0	-1
2	-1	0	-1	1
2	0	1	1	1
2	1	-1	1	0
2	1	1	-1	-1
3	-α	α	α	-α
3	0	0	0	0
3	0	0	0	0
3	0	0	0	0
3	α	-α	-α	α

(a)

Block	x1	x2	x3	x4
1	-1	-1	1	1
1	-1	1	-1	0
1	-1	1	1	-1
1	0	-1	-1	-1
1	0	0	0	0
1	1	-1	-1	1
1	1	0	1	-1
1	1	1	0	1
2	-α	-α	0	-α
2	-α	0	-α	α
2	0	0	0	0
2	0	0	0	0
2	0	α	α	α
2	α	-α	α	0
2	α	α	-α	-α

(b)

Figure 4: The 4-factor DSD used for the laser etch experiment (Jones & Nachtsheim, 2016) (a) in three orthogonal blocks, and (b) in two orthogonal blocks.

& Nachtsheim, 2016) (a) in three orthogonal blocks and (b) in two orthogonal blocks. In Figure 4 (a), α (= 1.4142) is the solution of the equation $\frac{2\alpha^2}{5} = \frac{4}{5}$ where 2 is the number of α's, 5 the size of each block and 4 the sum of squares contribution of each x_i, $(i = 1, \ldots, 4)$ for block 1 (and 2). In Figure 4 (b), α (= 1.1456) is the solution of the equation $\frac{4\alpha^2}{7} = \frac{6}{8}$ where 4 is the number of α's, 7 the size of the second block, 8 the size of the first block and 6 the sum of squares contribution of each x_i, $(i = 1, \ldots, 4)$ for block 1. Note that if α of the design in Figure 4 (a) is 1, the BF of this design will be 0.963 instead of 1. Also, if α of the design in Figure 4 (b) is 1, the BF of this design will be 0.993 instead of 1.

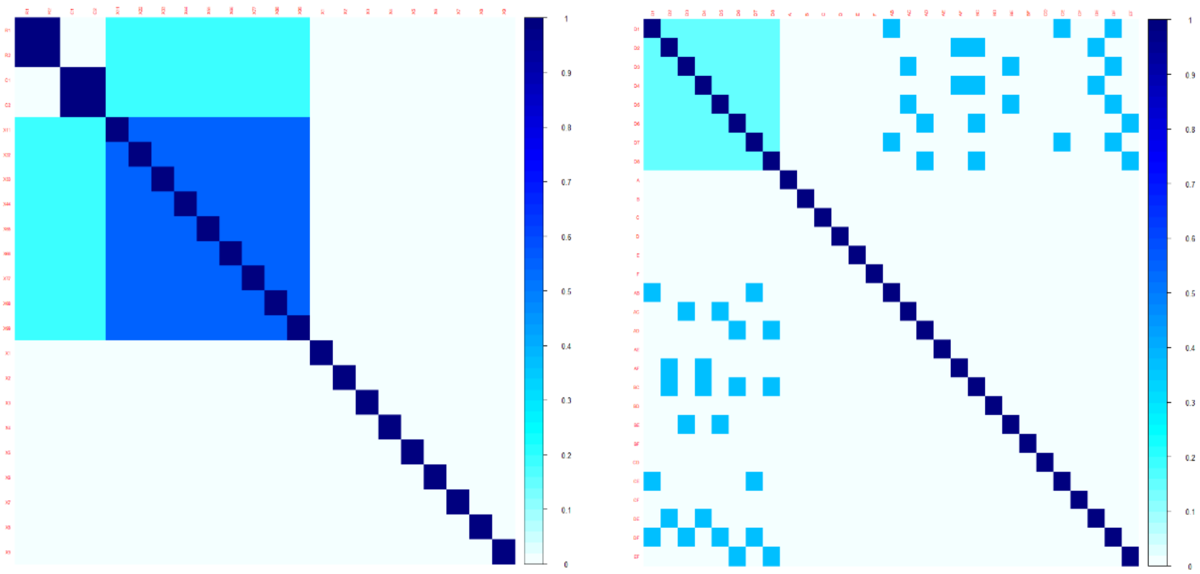
It is reasonable to compare a block design available in a catalog of block designs and that constructed by our blocking algorithm. Let's block a 2^{6-1} fractional factorial design (FFD) generated by the design generator **F**=**ABCDE** in eight blocks. To construct this block design, we can use the block generators **ACE**, **BCE** and **ADE** (See Table 5B.3 of

Block	A	B	C	D	E	F	Block	A	B	C	D	E	F
1	-1	1	-1	1	1	1	5	-1	-1	-1	-1	1	1
1	-1	1	1	-1	-1	-1	5	-1	1	-1	1	-1	-1
1	1	-1	-1	-1	1	-1	5	1	-1	1	1	1	-1
1	1	-1	1	1	-1	1	5	1	1	1	-1	-1	1
2	-1	-1	1	1	-1	-1	6	-1	-1	-1	1	1	-1
2	-1	1	-1	-1	1	-1	6	-1	1	1	1	-1	1
2	1	-1	1	-1	1	1	6	1	-1	-1	-1	-1	1
2	1	1	-1	1	-1	1	6	1	1	1	-1	1	-1
3	-1	-1	1	-1	-1	1	7	-1	-1	-1	1	-1	1
3	-1	1	1	1	1	-1	7	-1	-1	1	-1	1	-1
3	1	-1	-1	1	-1	-1	7	1	1	-1	-1	-1	-1
3	1	1	-1	-1	1	1	7	1	1	1	1	1	1
4	-1	-1	1	1	1	1	8	-1	-1	-1	-1	-1	-1
4	-1	1	-1	-1	-1	1	8	-1	1	1	-1	1	1
4	1	-1	1	-1	-1	-1	8	1	-1	-1	1	1	1
4	1	1	-1	1	1	-1	8	1	1	1	1	-1	-1

Figure 5: A 2^{6-1} fractional factorial arranged in eight blocks.

Wu & Hamada (2009)). The resulting design has clear main effects and 2fi's, except **AB**, **BC** and **CD**. In other words, these 2fi's are fully confounded with blocks and cannot be estimated. In contrast, our block design in Figure 5 has clear main effects and some clear 2fi's. Most 2fi's are however, partially confounded with blocks but can still be estimated.

To visualize the confounding patterns of block designs we use the correlation cell plots (CCPs). These CCPs, proposed by Jones & Nachtsheim (2011), display the magnitude of the correlation between main effects, quadratic effects of 3-level factors and 2fi's of the designs under study. The color of each cell in these plots ranges from white (no correlation) to dark (correlation of 1 or close to 1). Figure 6 (a) shows the confounding patterns of the 9-factor DSD in Figure 3. It can be seen from this CCP that the main effects of this design are clear of row/column effects. However, the quadratic effects are partially confounded with the block effects. Figure 6 (b) shows the confounding patterns of the 6-factor FFD in Figure 5. It can be seen from this CCP that the main effects of this design are clear of block effects. However, most 2fi's are partially confounded with the block effects.



(a) (b)

Figure 6: CCPs showing the confounding patterns of (a) a 9-factor DSD arranged in two rows and two columns, and (b) a 2^{6-1} fractional factorial arranged in eight blocks.

5 Conclusion

Most block designs in the literature are cataloged design and as such they are not flexible enough. The 2-level factorials and fractional factorials are only available in 2^q blocks, but not available in five, six or seven blocks. The 4-factor BBD, for example is available in three blocks but not in two blocks. Besides, catalogs do not offer designs having more than one blocking factor. Our blocking algorithm was developed with the philosophy "Design for experiment, not experiment for the design" in mind. We hope it could offer alternatives to the existing catalog of block designs. In the pre-computer age, the constructed block design strived for simplicity in the analysis. Nowadays, it is not simplicity in the analysis but the design efficiency and the saving of experimental resources that counts.

The supplemental material contains the Java implementation of the algorithm in Section 3. It also contain examples blocked factorial and fractional factorials, orthogonally blocked BBDs for 4-7 factors in rows and columns, some orthogonally blocked mixture designs in rows and columns, and some near-orthogonally blocked DSDs and DSD-based mixed-level designs (Jones & Nachtsheim, 2013) and Hadamard design-based mixed-level designs (Nguyen et al., 2019).

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