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TEMPLATES FOR DESIGN KEY CONSTRUCTION

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Abstract: We present some useful templates for implementing design key construction of factorial designs with simple block structures, in particular those for the construction of unblocked and blocked split-plot and strip-plot factorial designs. Constraints imposed by the block structure, additional requirements of the experiment, and some important information about the design are built into the template. These features add to the advantages of design key construction.

Key words and phrases: Block design, factorial design, row-column design, simple block structure, split-plot design, strip-plot design.

1. Introduction

The method of design key, proposed by Patterson (1965, 1976) (also see Patterson and Bailey (1978)), is a useful method of constructing designs for factorial experiments with what Nelder (1965a) called simple block structures. The simplest examples of simple block structures include, for instance, those of block designs (including split-plot designs) and row-column designs (including strip-plot designs). The design key method is applicable to symmetric or mixed-level designs. For s^n factorials where s is a prime number or power of a prime number, it is equivalent to the familiar method of using independent treatment factorial effects (words) to divide the treatment combinations into blocks, rows, and columns, etc. In the process of selecting the treatment words, certain conditions need to be verified to ensure that the desired block structure is achieved and some requirements imposed by the experiment are satisfied. The method of design key, on the other hand, guarantees the desired block structure by choosing some appropriate contrasts of the experimental units to be aliases of the main-effect contrasts of treatment factors. It has several advantages, including simple generation of the design layout and a unified construction for different block structures.

Patterson (1965, 1976) and Patterson and Bailey (1978) did not address the issue of how to choose design keys, and the same design can be produced by many different design keys. In this paper, for unblocked and blocked split-plot and strip-plot s^n factorial designs, where s is a prime number or power of a prime number, we present some useful templates to remove such redundancy so that efficient design searches can be performed and for implementing design key construction. Constraints imposed by the block structure and additional requirements of the experiment are built into the template.

To fix the ideas, in Sections 2 and 3 we first review the construction of blocked and row-column factorial designs, and present design key templates for these settings. After the construction and the relationship between the methods based on words and design keys are understood for the two simple cases, a general result is presented in Section 4. Design key templates for split-plot, blocked split-plot, and blocked strip-plot designs are derived in Sections 5, 6, and 7, respectively. We devote our discussions mostly to complete factorial designs. Modifications that are needed for fractional factorial designs are presented in Section 8.

2. Block Designs

In an s^n factorial experiment where s is a prime number or power of a prime number, each treatment combination can be represented by a vector $\boldsymbol{x} = (x_1, \ldots, x_n)^T$, with each $x_i \in \mathrm{GF}(s)$, the Galois field (finite field) with s elements. The set of all such vectors, s^n in total, is called the n-dimensional Euclidean geometry over $\mathrm{GF}(s)$. We refer the readers to Appendix A of Hinkelmann and Kempthorne (2005) for the definition of fields, and Chapter 11 there for detailed discussions of the construction of blocked factorial designs. To construct a complete s^n factorial design in s^q blocks of size s^{n-q}, a set of q linearly independent vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_q$ in $\mathrm{EG}(n, s)$ is chosen to perform the partition of the treatment combinations into blocks. Specifically, each block consists of the s^{n-q} vectors (treatment combinations) that are solutions of the q equations $\boldsymbol{a}_i^T \boldsymbol{x} = b_i$, $i = 1, \ldots, q$, where $b_i \in \mathrm{GF}(s)$. The q linearly independent vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_q$ are called independent blocking words. Under the constructed design, the $s - 1$ degrees of freedom defined by each nonzero linear combination of $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_q$ are confounded with block contrasts. We call the nonzero linear combinations of $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_q$ blocking words. Typically we avoid confounding the treatment main effects with block contrasts.

The s^q blocks can be determined as follows. We first solve the equations $\boldsymbol{a}_i^T \boldsymbol{x} = 0$, $i = 1, \ldots, q$, to obtain the principal block. Given s^k blocks ($k < q$) that have been obtained, pick a treatment combination $\boldsymbol{x}$ that has not appeared yet. Add each of the $s - 1$ nonzero multiples of $\boldsymbol{x}$ ($\lambda \boldsymbol{x}$ with $\lambda \in \mathrm{GF}(s)$, $\lambda \neq 0$) to all the treatment combinations in the s^k blocks to form $(s-1)s^k$ additional blocks. Then repeat the same procedure until s^q blocks are obtained. It follows that the design is completely determined by the principal block.

For design key construction, we note that the s^n experimental units can be thought of as all the combinations of an s^q-level factor $\mathcal{B}$ and an s^{n-q}-level factor $\mathcal{P}$, with the jth unit in the ith block represented by the combination where $\mathcal{B}$ is at level i and $\mathcal{P}$ is at level j. The (s^n-1)-dimensional space of unit contrasts can be decomposed as the direct sum of an (s^q-1)-dimensional space of block contrasts, called the interblock stratum, and an $s^q(s^{n-q}-1)$-dimensional space of within-block contrasts, called the intrablock stratum. It can be seen that the interblock stratum is the same as the space of the main-effect contrasts of $\mathcal{B}$, and the intrablock stratum is generated by the main-effect contrasts of $\mathcal{P}$ and the interaction contrasts of $\mathcal{B}$ and $\mathcal{P}$. Each treatment factorial effect (main effect or interaction) that coincides with a unit contrast representing the main effect of $\mathcal{B}$ (the latter is called the unit alias of the former) is confounded with a block contrast. On the other hand, if the unit alias of a treatment factorial effect is either the main effect of $\mathcal{P}$ or interaction of $\mathcal{B}$ and $\mathcal{P}$, then it is orthogonal to the block contrasts. If a design is constructed in such a way that each treatment main-effect contrast coincides with a unit contrast representing either the main effect of $\mathcal{P}$ or interaction of $\mathcal{B}$ and $\mathcal{P}$, then all the treatment main effects are orthogonal to block contrasts. Unit aliases of all treatment interactions can be obtained from those of the main-effect contrasts to determine whether they are orthogonal to or are confounded with block contrasts.

For convenience, we represent each of the s^q blocks by a combination of q s-level pseudo factors $\mathcal{B}_1, \ldots, \mathcal{B}_q$ and each of the s^{n-q} levels of $\mathcal{P}$ by a combination of $n-q$ s-level pseudo factors $\mathcal{P}_1, \ldots, \mathcal{P}_{n-q}$. Then each experimental unit can be represented by a combination $(p_1, \ldots, p_{n-q}, b_1, \ldots, b_q)^T$ of the levels of $\mathcal{P}_1, \ldots, \mathcal{P}_{n-q}, \mathcal{B}_1, \ldots, \mathcal{B}_q$. We call these n factors unit factors. A factorial effect of these factors falls in the interblock (respectively, intrablock) stratum if and only if it involves none (respectively, at least one) of the $\mathcal{P}_j$'s. Let $\boldsymbol{Y}$ be an $n \times s^n$ matrix with each row corresponding to a unit factor and each column corresponding to an experimental unit such that each column of $\boldsymbol{Y}$ is the corresponding level combination of the unit factors. Let

$$\boldsymbol{X} = \boldsymbol{K}\boldsymbol{Y}, \tag{2.1}$$

where $\boldsymbol{K}$ is a nonsingular $n \times n$ matrix with entries from GF(s). A design is obtained by assigning the treatment combination represented by the jth column of $\boldsymbol{X}$, $1 \leq j \leq s^n$, to the unit corresponding to the jth column of $\boldsymbol{Y}$. The nonsingularity of $\boldsymbol{K}$ is to ensure that all the s^n treatment combinations are generated.

By (2.1), each treatment combination $(x_1, \ldots, x_n)^T$ assigned to the experimental unit $(p_1, \ldots, p_{n-q}, b_1, \ldots, b_q)^T$ satisfies

$$x_i = \sum_{j=1}^{n-q} k_{ij} p_j + \sum_{l=1}^{q} k_{i,n-q+l} b_l;$$

that is, the factorial effect of the unit factors defined by the ith row of $\boldsymbol{K}$ is the unit alias of the main effect of the ith treatment factor. Thus the main effect of the ith treatment factor is orthogonal to the block contrasts if and only if at least one of $k_{i,1}, \ldots, k_{i,n-q}$ is nonzero. We call $\boldsymbol{K}$ a design key matrix. (Note that in Patterson (1976), $\boldsymbol{K}^T$ is called a key matrix.) Each row of $\boldsymbol{K}$ corresponds to a treatment factor and each of its columns corresponds to a unit factor. In practice, it is not necessary to perform the matrix multiplication in (2.1) to obtain the design layout. Let $\boldsymbol{e}_i$ be the $n \times 1$ vector whose ith entry is equal to 1 and all other entries equal to zero. Then $\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n\}$ is a set of independent generators of the s^n units. Suppose we generate and arrange the s^n units in the following Yates order with respect to $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n$: the first unit is $\mathbf{0}$ in which all the unit factors are at level 0; given that s^k units $(0 \leq k < n)$ have been generated, follow these units by $s - 1$ sets of size s^k, where each set is obtained by adding a nonzero multiple of $\boldsymbol{e}_{k+1}$ to the s^k units that have been generated. Continue until all the units are generated. Then the first s^{n-q} units in the generated sequence are in the same block, and each succeeding set of s^{n-q} units are also in the same block. Since $\boldsymbol{K}$ is nonsingular, $\boldsymbol{K}\boldsymbol{e}_1, \ldots, \boldsymbol{K}\boldsymbol{e}_n$, which are the columns of $\boldsymbol{K}$, give a set of independent generators of the treatment combinations. If we generate the treatment combinations using the generators $\boldsymbol{K}\boldsymbol{e}_1, \ldots, \boldsymbol{K}\boldsymbol{e}_n$, and arrange them in the same Yates order, then the first s^{n-q} treatment combinations in the generated sequence are in the same block, and each succeeding set of s^{n-q} treatment combinations are also in the same block.

Example 1. A 2^4 design in four blocks of size four, where the treatment factors are denoted by A, B, C, D, is constructed by using the two three-factor interactions ABC and ABD as independent blocking words.

(1)	c	d	cd
acd	ad	ac	a
bcd	bd	bc	b
ab	abc	abd	$abcd$

Note that we have used the convention of representing each treatment combination by a string of lower case letters; a letter is present if and only if the corresponding factor is at level 1. The first block consists of the four treatment combinations that have even numbers of letters in common with both ABC and ABD, where (1) is the combination with all the treatment factors at level 0. The other blocks can be obtained by repeating the process of symbolically multiplying the treatment combinations that have been generated by one that has not appeared yet, subject to the rule that the square of any letter is eliminated. This design can also be constructed by using $\mathcal{P}_1, \mathcal{P}_2, \mathcal{P}_1\mathcal{P}_2\mathcal{B}_1, \mathcal{P}_1\mathcal{P}_2\mathcal{B}_2$ as the unit aliases of the treatment main effects A, B, C, D, respectively. Since all these unit aliases involve at least one of $\mathcal{P}_1$ and $\mathcal{P}_2$, no treatment main effect is confounded with a block contrast. We have the following design key, where the unit alias of each treatment main effect is used to write down a row:

$$\boldsymbol{K} = \begin{array}{c} \begin{array}{cccc} \mathcal{P}_1 & \mathcal{P}_2 & \mathcal{B}_1 & \mathcal{B}_2 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{bmatrix} \end{array} \begin{array}{c} \\ A \\ B \\ C \\ D \end{array} \tag{2.2}$$

The design layout can be obtained by using the four independent generators acd, bcd, c, and d identified from the columns of $\boldsymbol{K}$. We start with (1) and the first generator acd. Multiplying them by the second generator bcd, we obtain the four treatment combinations in the first block. The second block can be obtained from the third generator c, and the last two blocks can be obtained from the fourth generator d. The unit aliases of ABC and ABD are $\mathcal{P}_1\mathcal{P}_2(\mathcal{P}_1\mathcal{P}_2\mathcal{B}_1) = \mathcal{B}_1$ and $\mathcal{P}_1\mathcal{P}_2(\mathcal{P}_1\mathcal{P}_2\mathcal{B}_2) = \mathcal{B}_2$, respectively. Since these unit aliases involve neither $\mathcal{P}_1$ nor $\mathcal{P}_2$, ABC and ABD are indeed blocking words. This can also be seen from the inverse of $\boldsymbol{K}^{-1}$:

$$\boldsymbol{K}^{-1} = \begin{array}{c} \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{bmatrix} \end{array} \begin{array}{c} \\ \mathcal{P}_1 \\ \mathcal{P}_2 \\ \mathcal{B}_1 \\ \mathcal{B}_1 \end{array}$$

In the inverse key matrix, which happens to be equal to $\boldsymbol{K}$, the roles of treatment and unit factors are reversed. From the last two rows, we can see that the treatment aliases of $\mathcal{B}_1$ and $\mathcal{B}_2$ are, respectively, the two independent blocking words ABC and ABD.

A method of constructing blocked s^n complete factorial designs proposed by Das (1964) and Cotter (1974), although not presented in the form of a design key, is essentially equivalent to using a design key of the form

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \boldsymbol{0}_{n-q,q} \\ \boldsymbol{B} & \boldsymbol{I}_q \end{bmatrix}, \tag{2.3}$$

where $\boldsymbol{I}$ is an identity matrix and $\boldsymbol{0}_{n-q,q}$ is the $(n-q)\times q$ matrix of 0's. The discussion in Example 1 shows that the principal block is generated by the first $n-q$ columns of $\boldsymbol{K}$. Since the principal block itself is an s^{n-q} fractional factorial design, it can be generated by using $n-q$ basic factors; that is, there are $n-q$ treatment factors such that the principal block contains each of their level combinations exactly once, and the other q treatment factors can be defined in terms of interactions of the basic factors. Thus there exists a set of $n-q$ independent generators of the principal block such that each basic factor appears at level 1 in exactly one of the generators and level 0 in all the other generators. Without loss of generality (subject to a relabeling of the treatment factors), we can assume that these basic factors correspond to the first $n-q$ rows of $\boldsymbol{K}$. Then the first $n-q$ columns of $\boldsymbol{K}$ are as shown in (2.3). On the other hand, since the design is completely determined by the principal block, we can choose the last q columns of $\boldsymbol{K}$ arbitrarily as long as $\boldsymbol{K}$ is nonsingular. Clearly the columns of $\boldsymbol{K}$ in (2.3) are linearly independent. Thus all block designs can be constructed by using a design key of the form in (2.3). If no treatment main effects are to be confounded with blocks, then all the rows of $\boldsymbol{B}$ must be nonzero. This gives a template for constructing blocked complete factorial designs. To choose a blocking scheme, only the q nonzero rows of $\boldsymbol{B}$ need to be chosen.

For a matrix of the from in (2.3), we have

$$\boldsymbol{K}^{-1} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \boldsymbol{0}_{n-q,q} \\ -\boldsymbol{B} & \boldsymbol{I}_q \end{bmatrix}, \tag{2.4}$$

in particular, for two-level designs, $\boldsymbol{K}^{-1} = \boldsymbol{K}$. It follows that each of the last q rows of $\boldsymbol{K}$ with the first $n-q$ components replaced by their additive inverses (unchanged when $s=2$) defines a treatment factorial effect that is confounded with block contrasts. It is clear that these rows are linearly independent. Thus the selection of q independent blocking words is equivalent to that of the q rows of $\boldsymbol{B}$, and a set of independent blocking words can be identified directly from the last q rows of $\boldsymbol{K}$. In comparison with the method based on words, we point out the advantages of not having to check independence of the blocking words, not having to check that no main effect is a generalized interaction of the independent blocking words, and not having to solve equations to identify the treatment combinations in the principal block. All of these are built into the template.

Example 2. (Example 1 revisited) By (2.3), a design key template is

$$\boldsymbol{K} = \begin{array}{cc} & \begin{array}{cccc} \mathcal{P}_1 & \mathcal{P}_2 & \mathcal{B}_1 & \mathcal{B}_2 \end{array} \\ & \left[\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ * & * & 1 & 0 \\ * & * & 0 & 1 \end{array}\right] \begin{array}{c} A \\ B \\ C \\ D \end{array} \end{array}$$

There are four unfilled entries, where at least one of the two unfilled entries in the same row must be 1. Suppose we fill all the four entries with 1. Then we have the design key in (2.2). The two independent blocking words ABC and ABD can be read directly from the last two rows of $\boldsymbol{K}$.

3. Row-column Designs

We refer the readers to Section 9.8 of Hinkelmann and Kempthorne (2005) for a discussion of the construction of row-column designs for two-level factorial experiments. To construct a complete s^n factorial row-column design with s^p rows and s^q columns, where $p + q = n$ and s is a prime number or power of a prime, we choose a set of $p+q$ linearly independent vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_p$, $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_q$ in $\mathrm{EG}(n, s)$. The s^n treatment combinations $\boldsymbol{x}$ are partitioned into s^p rows and s^q columns according to the values of $\boldsymbol{a}_i^T\boldsymbol{x}$, $i = 1, \ldots, p$, and $\boldsymbol{b}_j^T\boldsymbol{x}$, $j = 1, \ldots, q$, respectively. In this case the $(s^n - 1)$-dimensional space of unit contrasts is orthogonally decomposed into three strata: an $(s^p - 1)$-dimensional row stratum of row contrasts, an $(s^q - 1)$-dimensional column stratum of column contrasts, and an $(s^p - 1)(s^q - 1)$-dimensional unit stratum of those that are orthogonal to row and column contrasts. The treatment factorial effects defined by nonzero linear combinations of $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_p$ are confounded with row contrasts, and those defined by nonzero linear combinations of $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_q$ are confounded with column contrasts.

For design key construction, each unit is a combination of $n = p + q$ s-level pseudo factors $\mathcal{R}_1, \ldots, \mathcal{R}_p$ and $C_1, \ldots, C_q$. The main-effect and interaction contrasts of $\mathcal{R}_1, \ldots, \mathcal{R}_p$ are in the row-stratum, the main-effect and interaction contrasts of $C_1, \ldots, C_q$ are in the column-stratum, and the remaining interaction contrasts of $\mathcal{R}_1, \ldots, \mathcal{R}_p$ and $C_1, \ldots, C_q$ are in the unit stratum. Similar to the construction of block designs, the design key $\boldsymbol{K}$ is an $n \times n$ matrix with each row corresponding to a treatment factor and each column corresponding to one of the n unit factors $\mathcal{R}_1, \ldots, \mathcal{R}_p, C_1, \ldots, C_q$. We order the columns of $\boldsymbol{K}$ so that the first q correspond to $C_1, \ldots, C_q$ and the last p correspond to $\mathcal{R}_1, \ldots, \mathcal{R}_p$. The design generated by the first q columns of $\boldsymbol{K}$ is an s^{n-p} fractional factorial design, and that generated by the last p columns is an s^{n-q} fractional factorial design. The former has a set A_2 of q basic factors and the latter has a set A_1 of p basic factors. Since a complete s^n factorial is generated by the n columns together, A_1 and A_2 can be chosen to be disjoint. Let the first q rows of $\boldsymbol{K}$ correspond to those in A_2 and the last p rows correspond to those in A_1. Then without loss of generality (subject to treatment factor relabeling), we can use a design key matrix of the form

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_q & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{I}_p \end{bmatrix}. \tag{3.1}$$

If no treatment main-effect contrasts are to be confounded with row or column contrasts, then all the rows of $\boldsymbol{B}$ and $\boldsymbol{C}$ must be nonzero. This gives a design key template for complete factorial row-column designs. Again it can be seen that selection of the n independent words $\boldsymbol{a}_1, \cdots, \boldsymbol{a}_p, \boldsymbol{b}_1, \cdots, \boldsymbol{b}_q$ is equivalent to that of the n rows of $\boldsymbol{B}$ and $\boldsymbol{C}$. The design layout can be obtained by generating the treatment combinations from the columns of $\boldsymbol{K}$ in the Yates order. Each succeeding set of s^q treatment combinations from the beginning of the generated sequence yields one row of the design, with the treatment combinations in each set assigned to the columns in the order as given.

Under a strip-plot design (see, e.g., Miller (1997)), some treatment factors, called row treatment factors, must have constant level on all the units in the same row, and the other treatment factors, called column treatment factors, must have constant level on all the units in the same column. The main effects of row treatment factors are confounded with row contrasts and those of column treatment factors are confounded with column contrasts. For complete factorial strip-plot designs with p row treatment factors and q column treatment factors, the first q rows of the design key $\boldsymbol{K}$ in (3.1) correspond to column treatment factors, the last p rows correspond to row treatment factors, and both $\boldsymbol{B}$ and $\boldsymbol{C}$ must be zero matrices. In other words, we have the design key

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_q & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I}_p \end{bmatrix}. \tag{3.2}$$

In this case, the design is completely determined by the design for the row treatment factors, called the row design, and that for the column treatment factors, called the column design. Specifically, the strip-plot design is the product of the row design and column design: each combination of the row treatment factors is coupled with each combination of the column treatment factors once.

4. A General Result

Under a block design, a set of unstructured units is nested in each of another set of unstructured units. On the other hand, the block structure of a row-column design involves the crossing of two sets of unstructured units. Nelder (1965a) defined simple block structures to be those that can be obtained by repeated nesting and crossing. McLeod and Brewster (2004) considered blocking of factorial split-plot designs, where there are two layers of nesting: subplots are nested in whole-plots, which in turn are nested in blocks. The blocked strip-plot designs considered by Miller (1997) have a block structure that is obtained by combining nesting with crossing: a row-column structure is nested in each of several blocks. Both blocked split-plot and blocked strip-plot designs have block structures that are examples of a simple block structure. Analysis of randomized experiments with simple block structures and rules for determining the strata can be found in Nelder (1965a,b).

Similar to the derivation of (2.3) and (3.1), the following result can easily be established.

Theorem 1. *Let $\mathfrak{B}_1$ and $\mathfrak{B}_2$ be simple block structures on s^{m_1} and s^{m_2} units, respectively, where s is a prime number or power of a prime number, $n = m_1+m_2$, and $\mathfrak{B}_1/\mathfrak{B}_2$ (respectively, $\mathfrak{B}_1 \times \mathfrak{B}_2$) be block structures on s^n units obtained by nesting $\mathfrak{B}_2$ in $\mathfrak{B}_1$ (respectively, crossing $\mathfrak{B}_1$ and $\mathfrak{B}_2$). Without loss of generality, a design key $\boldsymbol{K}$ for a complete s^n factorial with block structure $\mathfrak{B}_1/\mathfrak{B}_2$ or $\mathfrak{B}_1 \times \mathfrak{B}_2$ can be expressed as*

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{K}_2 & \boldsymbol{A} \\ \boldsymbol{B} & \boldsymbol{K}_1 \end{bmatrix} \tag{4.1}$$

for some matrices $\boldsymbol{A}$ and $\boldsymbol{B}$, where $\boldsymbol{K}_1$ is a design key for a complete s^{m_1} factorial with block structure $\mathfrak{B}_1$ and $\boldsymbol{K}_2$ is a design key for a complete s^{m_2} factorial with block structure $\mathfrak{B}_2$, the first m_2 columns of $\boldsymbol{K}$ correspond to the unit factors in $\mathfrak{B}_2$ and the last m_1 columns correspond to the unit factors in $\mathfrak{B}_1$. Furthermore, if the s^{m_1} units in $\mathfrak{B}_1$ are unstructured, then a design key for a complete s^n factorial with the block structure $\mathfrak{B}_1/\mathfrak{B}_2$ can be expressed as

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{K}_2 & \boldsymbol{0} \\ \boldsymbol{B} & \boldsymbol{I}_{m_1} \end{bmatrix}. \tag{4.2}$$

As an application of Theorem 1, we derive design key templates for blocked split-plot and strip-plot designs in Sections 6 and 7, respectively.

5. Split-plot Designs

Consider the construction of s^n complete factorial split-plot designs with s^q whole-plots each containing s^{n-q} subplots, where n_1 of the n treatment factors are whole-plot factors and the other $n_2 = n - n_1$ treatment factors are subplot factors. For complete factorials, we must have $n_1 \le q$. The results in Section 2 can be applied to the current setting since the block structure of a split-plot design is the same as that of a block design, with the whole-plots and subplots playing the same roles of blocks and units, respectively. Denote $\mathcal{P}_1, \ldots, \mathcal{P}_{n-q}$ and $\mathcal{B}_1, \ldots, \mathcal{B}_q$ in Section 2 by $\mathcal{S}_1, \ldots, \mathcal{S}_{n-q}$ and $\mathcal{W}_1, \ldots, \mathcal{W}_q$, respectively; here $\mathcal{S}_1, \ldots, \mathcal{S}_{n-q}$ define the subplots in each whole-plot, and $\mathcal{W}_1, \ldots, \mathcal{W}_q$ define the whole-plots. We can use a design key $\boldsymbol{K}$ of the form in (2.3), where $\boldsymbol{B}$ is $q \times (n-q)$, the first $n-q$ columns of $\boldsymbol{K}$ correspond to $\mathcal{S}_1, \ldots, \mathcal{S}_{n-q}$, and the last q columns correspond to $\mathcal{W}_1, \ldots, \mathcal{W}_q$. In this setting, the interblock and intrablock strata are called, respectively, whole-plot and subplot strata.

Since the unit alias of the main effect of each whole-plot treatment factor cannot involve any of $\mathcal{S}_1, \ldots, \mathcal{S}_q$, each row of $\boldsymbol{K}$ that corresponds to a whole-plot treatment factor must have all the first $n-q$ components equal to zero. Thus, unlike in Section 2, there is an additional constraint that the first $n-q$ rows of $\boldsymbol{K}$ must correspond to subplot treatment factors. Without loss of generality, let the next n_1 rows correspond to whole-plot treatment factors and, if $n_1 < q$, the last $q - n_1$ rows correspond again to subplot treatment factors. Then all the first n_1 rows of $\boldsymbol{B}$ must be zero and, if $n_1 < q$, the last $q - n_1$ rows of $\boldsymbol{B}$ are nonzero. This gives a template for constructing complete s^n factorial split-plot designs.

For $n_1 < q$, the design key construction requires the selection of $q - n_1$ nonzero rows of $\boldsymbol{B}$. This is the case where the number of whole-plot treatment factor level combinations is less than the number of whole-plots, and hence the design on the whole-plots consists of s^{q-n_1} copies of the complete factorial of whole-plot treatment factors. The construction in Bingham, Schoen, and Sitter (2004) uses $q - n_1$ independent splitting words to partition each of s^{n_1} sets of subplot treatment factor combinations that are coupled with the same whole-plot treatment factor combination into s^{q-n_1} smaller sets, resulting in a total of $s^{n_1} \cdot s^{q-n_1} = s^q$ whole-plots. The splitting words (splitting effects) are factorial effects that involve some subplot treatment factors but are confounded with whole-plot contrasts. The selection of the last $q - n_1$ rows of $\boldsymbol{B}$ is equivalent to that of independent splitting words, and these words can be identified from the last $q - n_1$ rows of $\boldsymbol{K}$ in the same way as the determination of independent blocking words in Section 2.

Two further advantages, in addition to those mentioned in Section 2, are that it is not necessary to go through the splitting process and that one single design key works for all the situations regardless of whether $n_1 = q$ or $n_1 < q$.

6. Blocked Split-plot Designs

Consider the construction of an s^n complete factorial split-plot design with s^q whole-plots each containing s^{n-q} subplots, where there are n_1 whole-plot treatment factors, $n_2 = n - n_1$ subplot treatment factors, and the s^q whole-plots are divided into s^g blocks each of size s^{q-g}. McLeod and Brewster (2004) presented three methods (pure whole-plot blocking, separation, and mixed blocking) for constructing blocked split-plot designs. We show that one single template is sufficient to generate the designs in a simple manner in all the situations. McLeod and Brewster's (2004) three methods are more complicated and do not cover all the cases.

In the current setting the $(s^n - 1)$-dimensional space of unit contrasts is orthogonally decomposed into an $(s^g - 1)$-dimensional space of block contrasts, called the block stratum, an $s^g(s^{q-g} - 1)$-dimensional space of whole-plot contrasts within the same block, called the whole-plot stratum, and an $s^q(s^{n-q} - 1)$-dimensional space of between-subplot contrasts within the same whole-plot, called the subplot stratum. Each experimental unit can be represented by a combination of $n = (n - q) + (q - g) + g$ unit factors $\mathcal{S}_1, \ldots, \mathcal{S}_{n-q}, \mathcal{W}_1, \ldots, \mathcal{W}_{q-g}, \mathcal{B}_1, \cdots, \mathcal{B}_g$; here $\mathcal{S}$, $\mathcal{W}$, and $\mathcal{B}$ stand for subplots, whole-plots and blocks, respectively. A treatment main effect is confounded with a block (respectively, whole-plot) contrast if its unit alias does not involve any of $\mathcal{S}_1, \ldots, \mathcal{S}_{n-q}, \mathcal{W}_1, \ldots, \mathcal{W}_{q-g}$ (respectively, involves at least one of $\mathcal{W}_1, \ldots, \mathcal{W}_{q-g}$ but not any of $\mathcal{S}_1, \ldots, \mathcal{S}_{n-q}$), and is orthogonal to block and whole-plot contrasts if its unit alias involves at least one of $\mathcal{S}_1, \ldots, \mathcal{S}_{n-q}$.

Throughout the rest of this section, we assume that the between-whole-plot variance within the same block is less than the between-block variance. This is often the case in practice, and can be shown to hold under the usual mixed-effect model for blocked split-plot designs; see, e.g., (2.10) of Cheng and Tsai (2011). Under this assumption, if $n_1 \leq q - g$ (that is, the number of whole-plot treatment factor level combinations is no more than the number of whole-plots in each block), then in each block it is better to have all the whole-plot treatment factor level combinations appear the same number of times than to have a replicated fractional factorial of the whole-plot treatment factors. On the other hand, if $n_1 > q - g$, then in each block it is better to have an unreplicated $s^{n_1-(n_1-q+g)}$ design for the whole-plot treatment factors than replications of a more fractionated design. A theorem provides a design key template for blocked split-plot designs.

Theorem 2. *Suppose no treatment main effects are confounded with block contrasts, no replication of the same whole-plot treatment factor level combination in each block is allowed when $n_1 \geq q-g$, and the within-block replication is minimized when $n_1 < q-g$. Then, without loss of generality, we have a design key template for blocked split-plot designs:*

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \boldsymbol{0}_{n-q,q-g} & \boldsymbol{0}_{n-q,g} \\ \multirow{2}{*}{$\boldsymbol{B}$} & \boldsymbol{I}_{q-g} & \boldsymbol{0}_{q-g,g} \\ & \boldsymbol{C} & \boldsymbol{I}_g \end{bmatrix}, \tag{6.1}$$

where $\boldsymbol{B}$ is $q \times (n-q)$, $\boldsymbol{C}$ is $g \times (q-g)$, the first $n-q$ columns of $\boldsymbol{K}$ correspond to $\mathcal{S}_1, \ldots, \mathcal{S}_{n-q}$, the next $q-g$ columns correspond to $\mathcal{W}_1, \ldots, \mathcal{W}_{q-g}$, the last g columns correspond to $\mathcal{B}_1, \ldots, \mathcal{B}_g$, the first $n-q$ rows of $\boldsymbol{K}$ correspond to subplot treatment factors, the next n_1 rows correspond to whole-plot treatment factors, and all the remaining rows correspond to subplot treatment factors if $n_1 < q$. Furthermore, the first n_1 rows of $\boldsymbol{B}$ are zero, all the last $q-n_1$ rows of $\boldsymbol{B}$ are nonzero if $n_1 < q$, and all the first $n_1-(q-g)$ rows of $\boldsymbol{C}$ are nonzero if $n_1 > q-g$.

Proof. Since we have a block structure wherein s^{q-g} whole-plots, each containing s^{n-q} subplots, are nested in each of s^g blocks, (4.2) in Theorem 1 is applicable. We have $m_1 = g$, and the matrix $\boldsymbol{K}_2$ in (4.2) can be obtained from (2.3), with q replaced by $q-g$. Thus without loss of generality, we have a design key of the form

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{B}_1 & \boldsymbol{I}_{q-g} & \boldsymbol{0} \\ \boldsymbol{B}_2 & \boldsymbol{C} & \boldsymbol{I}_g \end{bmatrix}.$$

Since all the rows of $\boldsymbol{I}_{n-q}$ are nonzero, the first $n-q$ rows of $\boldsymbol{K}$ must correspond to subplot treatment factors.

The columns of $\boldsymbol{K}$ corresponding to those of $\boldsymbol{I}_{q-g}$ in the middle are used to generate the whole-plot treatment factor combinations in the first block. If $n_1 \geq q-g$ and no whole-plot treatment factor combination is replicated in each block as required, then the treatment combinations generated by these $q-g$ columns can also be generated by using a certain set of $q-g$ whole-plot treatment factors as basic factors. Without loss of generality, we can associate these factors with the rows of $\boldsymbol{K}$ that correspond to those of $\boldsymbol{B}_1$. Then all the entries of $\boldsymbol{B}_1$ are zero. If $n_1 > q-g$, then $n_1-(q-g)$ of the last g rows of $\boldsymbol{K}$ must also correspond to whole-plot treatment factors. Without loss of generality, take these to be the first $n_1 - (q-g)$ of the last g rows of $\boldsymbol{K}$. Then the corresponding rows of $\boldsymbol{B}_2$ (respectively, $\boldsymbol{C}$) must be zero (respectively, nonzero). The assertion about $\boldsymbol{C}$ follows from the constraint that no treatment main effects are confounded with block contrasts. The last $q - n_1$ rows of $\boldsymbol{K}$ correspond to subplot treatment factors, and hence the corresponding rows of $\boldsymbol{B}_2$ are nonzero.

Similarly, if $n_1 < q - g$ and within-block replication of whole-plot treatment factor combinations is to be kept at the minimum, then the treatment combinations generated by the $q - g$ columns of $\boldsymbol{K}$ corresponding to those of $\boldsymbol{I}_{q-g}$ can be generated by using a certain set of n_1 whole-plot treatment factors and $q - g - n_1$ subplot treatment factors as basic factors. Without loss of generality, we can associate the rows of $\boldsymbol{K}$ that correspond to the first n_1 rows of $\boldsymbol{B}_1$ with whole-plot treatment factors and associate the last $q - n_1$ rows of $\boldsymbol{K}$ with subplot treatment factors. Then the first n_1 rows of $\boldsymbol{B}_1$ are zero, and the remaining rows of $\boldsymbol{B}_1$ as well as all the rows of $\boldsymbol{B}_2$ are nonzero. This completes the proof.

If $n_1 \geq q - g$, then the design key matrix in (6.1) reduces to

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I}_{q-g} & \mathbf{0} \\ \boldsymbol{B}_2 & \boldsymbol{C} & \boldsymbol{I}_g \end{bmatrix}.$$

In this case, as in Section 2,

$$\boldsymbol{K}^{-1} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I}_{q-g} & \mathbf{0} \\ -\boldsymbol{B}_2 & -\boldsymbol{C} & \boldsymbol{I}_g \end{bmatrix}, \tag{6.2}$$

and $\boldsymbol{K}^{-1} = \boldsymbol{K}$ for two-level designs. Thus each of the last g rows of $\boldsymbol{K}$ with the first $n - g$ components replaced by their additive inverses (unchanged when $s = 2$) defines a blocking effect. Furthermore, if $n_1 < q$, then the last $q - n_1$ of these blocking words (those that are determined from the last $q - n_1$ rows of $\boldsymbol{K}$) are also splitting words.

For $n_1 < q - g$, $\mathbf{K}^{-1}$ cannot be obtained from $\mathbf{K}$ by changing the signs of $\mathbf{B}$ and $\mathbf{C}$. This is also the case not covered by the three methods proposed by McLeod and Brewster (2004). Here, independent splitting words can be determined from the last $q - n_1$ rows of $\boldsymbol{K}^{-1}$, and the last g of these splitting words are also blocking words. Nevertheless, it can be seen that $q - n_1 - g$ independent splitting words that are not blocking words can still be determined in the same way as described before directly from the rows of $\boldsymbol{K}$ that correspond to those of the last $q - n_1 - g$ rows of $\boldsymbol{I}_{q-g}$.

7. Blocked Strip-plot Designs

As another application of Theorem 1, we present a design key template for blocked strip-plot designs. Consider the construction of a complete s^n factorial design with s^g blocks each containing s^{p+q} units that are arranged in s^p rows and s^q columns, where $n = p+q+g$. In this case the (s^n-1)-dimensional space of unit contrasts is orthogonally decomposed into an (s^g-1)-dimensional space of block contrasts, called the block stratum, an $s^g(s^p-1)$-dimensional space of row contrasts within the same block, called the row stratum, an $s^g(s^q-1)$-dimensional space of column contrasts within the same block, called the column stratum, and an $s^g(s^p-1)(s^q-1)$-dimensional unit stratum. Each experimental unit can be represented by a combination of $n = p + q + g$ unit factors $\mathcal{R}_1, \ldots, \mathcal{R}_p, C_1, \ldots, C_q, \mathcal{B}_1, \ldots, \mathcal{B}_g$; here $\mathcal{R}$, C, and $\mathcal{B}$ stand for rows, columns and blocks, respectively. A factorial effect of the unit factors is in the block (respectively, row, column, or unit) stratum if it involves only the $\mathcal{B}$'s (respectively, at least one $\mathcal{R}$ but no C's, at least one C but no $\mathcal{R}$'s, or at least one $\mathcal{R}$ and at least one C).

Suppose n_1 (respectively, $n_2 = n - n_1$) of the treatment factors are row (respectively, column) treatment factors. For complete factorial designs we must have $n_1 \geq p$ and $n_2 \geq q$. A design key can be obtained from (4.2) with $m_1 = g$ and $\boldsymbol{K}_2$ given by (3.2):

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_q & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I}_p & \mathbf{0} \\ \boldsymbol{A} & \boldsymbol{B} & \boldsymbol{I}_g \end{bmatrix}, \tag{7.1}$$

where the first q columns correspond to $C_1, \ldots, C_q$, the next p columns correspond to $\mathcal{R}_1, \ldots, \mathcal{R}_p$, and the last g columns correspond to $\mathcal{B}_1, \ldots, \mathcal{B}_g$, the first q rows correspond to column treatment factors, the next p rows correspond to row treatment factors, and the last g rows correspond to the remaining row or column treatment factors. For any of the last g rows that corresponds to a row (respectively, column) treatment factor, the corresponding row of $\boldsymbol{A}$ (respectively, $\boldsymbol{B}$) must be zero. A blocking word can be identified from each of the last g rows by using the rule described before.

Example 3. Miller (1997) constructed a 32-run blocked strip-plot design with four rows and four columns in each of two blocks, six two-level row treatment factors, and four two-level column treatment factors. We consider here the construction of a full factorial with three two-level row treatment factors (A, B, C) and two two-level column treatment factors (S, T), and return to the original fractional factorial setting of Miller (1997) in Section 8. By (7.1), we have a design key of the form

$$\begin{array}{cc} \begin{array}{ccccc} \mathcal{C}_1 & \mathcal{C}_2 & \mathcal{R}_1 & \mathcal{R}_2 & \mathcal{B} \end{array} & \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & * & * & 1 \end{bmatrix} & \begin{array}{c} S \\ T \\ A \\ B \\ C \end{array} \end{array}$$

Suppose we choose the two unfilled entries (from left to right) to be 1 and 0, respectively. Then the blocking word is AC. The design can be constructed by writing the 32 treatment combinations in the Yates order with respect to the generators identified from the five columns of the design key. The first two generators determine the first row in the first block, the next two generators complete the other rows in the first block, and the second block is obtained from the last generator.

8. Fractional Factorial Designs

For constructing an s^{n-h} fractional factorial design with the block structures discussed, we can add h rows to a design key for the complete factorial of $n-h$ basic factors, one for each added factor. Then two treatment factorial effects are aliased if and only if their unit aliases are aliased. Given the defining relation of the fraction, the row of the design key associated with each added factor can be obtained as a linear combination of the rows corresponding to the basic factors whose interaction is used to define the given factor. We need to check that the constraints imposed by the block structures are satisfied. For instance, in the setting of Section 2, if no treatment main effects are to be confounded with block contrasts, then one needs to make sure that at least one of the first $n-q$ entries of each of the added rows is nonzero.

We illustrate the method on the construction of fractional factorial blocked strip-plot designs. In the setting of Section 7, suppose there are n_1 row treatment factors, n_2 column treatment factors, $n_1 \geq p+g$, $n_2 \geq q+g$, and $n > p+q+g$, where $n = n_1 + n_2$. In this case, the row and column designs are blocked $s^{n_1-(n_1-p-g)}$ and $s^{n_2-(n_2-q-g)}$ designs, respectively. Miller's (1997) construction starts with the product of two such blocked designs, which produces a blocked strip-plot design with s^{2g} blocks. The construction is completed by suitably choosing s^g of the s^{2g} blocks. We show how the design can be constructed in a simple manner by using a design key.

Suppose the design key for the complete factorial of $p+q+g$ basic factors obtained in Section 7 has a rows corresponding to row treatment factors with the other $b = p+q+g-a$ rows corresponding to column treatment factors. If $a < p+g$, then we need to expand the a row treatment factors to a set of $p+g$ basic factors for the row design. Likewise, if $b < q+g$, then we need to expand the b column treatment factors to a set of $q+g$ basic factors for the column design. We use independent interactions of the basic factors for the row (respectively, column) design to define the other $n_1-(p+g)$ row treatment factors (respectively, $n_2-(q+g)$ column treatment factors). Altogether we need to define $(p+g-a)+(q+g-b) = g$ additional factors to serve as basic factors for the row and column designs. A lemma shows that each of the g blocking words is used to produce such a factor.

Lemma 1. *Suppose no replication of the same level combination is allowed in both the row and column designs. If $a < p+g$ (respectively, $b < q+g$), then each of the $p+g-a$ (respectively, $q+g-b$) additional basic factors for the row (respectively, column) design is defined by a word of the form XY, where X involves some of the a row treatment factors only, Y involves some of the b column treatment factors only, and both X and Y involve at least one factor. Furthermore, if XY defines a basic factor for the row design, then Y is a blocking word, and if it defines a basic factor for the column design, then X is a blocking word .*

Proof. Each of the additional basic factors for the row and column designs is defined by a word that involves both row and column treatment factors; otherwise we would not be able to generate s^{p+g} distinct row treatment factor combinations and s^{q+g} distinct column treatment factor combinations. Write such a word in the form XY. Then in the case where XY defines a basic factor for the row design, the unit alias of Y must not involve any of $C_1, \ldots, C_q$. Furthermore, since Y is an interaction of the column treatment factors, its unit alias also does not involve any of $\mathcal{R}_1, \ldots, \mathcal{R}_p$. Thus Y is a blocking word. A similar conclusion holds for the case in which XY defines a basic factor for the column design.

The conclusion of Lemma 1 has each additional basic factor for the row design defined by aliasing a row treatment interaction with a blocking word involving column treatment factors only. Likewise, each additional basic factor for the column design is defined by aliasing a column treatment interaction with a blocking word involving row treatment factors only. As a result, g independent defining words are created. Essentially this is equivalent to selecting s^g of the s^{2g} blocks in the product of a blocked row design and a blocked column design, as mentioned earlier.

Example 4. [Example 3 continued] Miller's (1997) example involved six row treatment factors A, B, C, D, E, F and four column treatment factors S, T, U, V. (Note that Miller (1997) denoted the column treatment factors as a, b, c, and d, respectively.) A design key for the basic factors A, B, C, S, T was obtained in Example 3. We already have a set of three basic factors A, B, C for the row design; so only an additional basic factor, say U, is needed for the column design. Since AC is the single blocking word for the basic design, by Lemma 1, we must define U by an interaction of the form ACX, where X is a factorial effect of S and T. Suppose we replace the two levels 0 and 1 with -1 and 1, respectively, and define U as ACS (another choice is $-ACST$; ACT would give an isomorphic design). Then the defining word $ACSU$ is introduced, so SU is also a blocking word. The design can be completed by choosing three independent interactions of A, B, and C to define D, E, and F, and one interaction of S, T, U to define V. Suppose D, E, and F are defined by $D = -AB$, $E = ABC$, $F = -BC$, and V is defined by $V = STU$. Then we have the design key matrix.

$$\boldsymbol{K} = \begin{array}{c} \begin{array}{ccccc} \mathcal{C}_1 & \mathcal{C}_2 & \mathcal{R}_1 & \mathcal{R}_2 & \mathcal{B} \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 \end{bmatrix} \end{array} \begin{array}{c} \\ S \\ T \\ A \\ B \\ C \\ D \\ E \\ F \\ U \\ V \end{array}.$$

The resulting design, which can be generated in a simple manner from the five columns of $\boldsymbol{K}$, is the same as that constructed by Miller (1997) after C and D are switched.

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