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On a construction procedure for split-block-plot designs based on the Khatri–Rao product of incidence matrices

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SUMMARY

The construction of incomplete split-block-plot (SBP) designs for three-factor experiments is investigated. A semi-Kronecker (Khatri–Rao) product of matrices is used in the construction procedure. With this method some generated designs are obtained where column treatments and subplot treatments are allocated in balanced square lattice designs, while row treatments are in a randomized complete block design. Experiments with an orthogonal block structure are considered. In this paper we consider designs which are generally balanced. This allows us to give the stratum efficiency factors for treatment combination contrasts in the proposed split-block-plot designs.

Key words: Generally balanced designs, Semi-Kronecker product of matrices, Square lattice designs, Split-block-plot designs, Stratum efficiency factors.

1. Introduction

The split-block-plot (SBP) design presented here, used in some agricultural three-factor experiments and in glasshouse trials, is a combination of a split-plot and a split-block design. Another term for it is the strip-split-plot design (e.g. Gomez and Gomez, 1984). We may note that the SBP design is an extension of the split-block design (for the first two factors) in which the intersection plot is divided into subplots to accommodate a third factor.

Experiment is the basic research tool in the experimental sciences. Hence, an extremely important issue is the optimal planning of experiments. We take into account both the statistical properties of the experiment, technical problems with its implementation, and its cost.

Here, we deal with both the optimal statistical properties of the experiment and the possible reduction of the cost of its implementation. Reduction of the cost of the experiment is obtained by selecting methods of experiment construction with favorable statistical properties, and using a smaller number of experimental units.

In this paper we consider a situation when the considered design is incomplete (in a certain sense, non-orthogonal) with respect to one or more factors. Generally, by incompleteness of the design we mean that the numbers of units (rows, columns and subplots) used in blocks to accommodate the factors can be less than the numbers of their levels. In this case we consider the situation where the row treatments or column treatments and subplot treatments are non-orthogonal to blocks.

The modelling and analysis of data obtained from such experiments are presented, inter alia, in papers by Ambroży and Mejza (2002) and Mejza and Ambroży (2003, 2004). The authors also considered constructions of incomplete SBP designs based on the Kronecker product of incidence matrices for subdesigns (for the row treatments, the column treatments and the subplot treatments; e.g. Ambroży and Mejza, 2002).

The purpose of this paper is to investigate the construction of incomplete SBP designs based on the semi-Kronecker product of matrices, also called the Khatri–Rao product (see Khatri and Rao, 1968; Rao and Mitra, 1971). This leads to designs with a lower number of experimental units. In this case the generating designs (for the row or column treatments and the subplot treatments) should possess a property of resolvability. This method was also presented in a paper by Mejza et al. (2020) for a design with a nested structure of the units only.

Resolvable designs (e.g. lattice designs, α-designs) are commonly used in practice for one- or two-factor experiments (see Cox, 1958; John and Williams, 1999). In this paper we use one such design, from the class of designs with an orthogonal block structure, to construct a new incomplete SBP design, that is, a system with a more complex block structure. The construction procedure is

discussed for the case when balanced square lattice designs are used for the row or column treatments and the subplot treatments.

2. Assumptions and notations

Consider an $(s \times t \times w)$ - factorial experiment in which the first factor, say A, has s levels $A_1, A_2, \ldots, A_s$, the second factor, say B, has t levels $B_1, B_2, \ldots, B_t$, and the third factor, say C, has w levels $C_1, C_2, \ldots, C_w$. Let v (= stw) be the number of all treatment combinations.

We assume that the experimental material is divided into b blocks. Every block forms a row–column design with k_1 rows and k_2 columns. Then each intersection plot (also called whole plot) is divided into k_3 subplots. Hence, the number of observations is equal to n $(= bk_1k_2k_3)$. Here the rows correspond to the levels of the factor A, also termed row treatments, the columns correspond to the levels of the factor B, also called column treatments, and the subplots serve to accommodate the levels of the factor C, termed subplot treatments. It may be noted that there are four plot sizes (the row, the column, the whole plot and the subplot), so there are possible four levels of precision with which the effects of the various factors are estimated. The highest level corresponds to the subplot factor levels and their interactions with other factor levels. The precision is strictly connected with the efficiency of the estimation of the contrasts (comparisons) of the treatment combinations.

In this paper we consider a situation when the SBP design with $k_1 = s$, $k_2 < t$, $k_3 < w$ is incomplete with respect to two factors only. Since all units have to be randomized before they enter the experiment, we perform four-step randomization. Let us note that the first three steps of the randomization connected with the blocks, the rows and the columns are strictly the same as in the split-block design, whereas the fourth step, connected with the subplots, takes place as in the split-plot design. This mixed process of randomization leads to a randomization model with five main strata (without the zero stratum related to

the mean of an experiment only). This model is of the form (Ambroży and Mejza, 2002):

$$\mathrm{E}(\mathbf{y}) = \boldsymbol{\Delta}'\boldsymbol{\tau}, \qquad \mathrm{Cov}(\mathbf{y}) = \mathbf{V}(\gamma), \tag{2.1}$$

where $\boldsymbol{\Delta}'$ is a known design matrix for v treatment combinations, and $\boldsymbol{\tau}$ ($v\times1$) is the vector of fixed treatment combination effects. According to the orthogonal block structure of SBP designs, the dispersion matrix $\mathbf{V}(\gamma)$ can be expressed by $\mathbf{V}(\gamma) = \sum_{f=0}^{5} \gamma_f \mathbf{P}_f$, where $\gamma_f \geq 0$ and $\{\mathbf{P}_f\}$ are a family of known pairwise orthogonal projectors adding to the identity matrix (Houtman and Speed, 1983). The range space $\Re\{\mathbf{P}_f\}$ of $\mathbf{P}_f$, f = 0, 1,.., 5, is termed the f-th stratum of the model, and $\{\gamma_f\}$ are unknown strata variances. This model will be analyzed using the methods developed for multistratum experiments (Nelder, 1965a and 1965b). Thus, we have a zero stratum (0) generated by the vector of ones, an inter-block stratum (1), an inter-row (within the block) stratum (2), an inter-column (within the block) stratum (3), an inter-whole plot (within the block) stratum (4), and an inter-subplot (within the whole plot) stratum (5).

The considered SBP designs will be characterized with respect to stratum efficiencies for chosen groups of contrasts among treatment combination effects, with regard to the general balance property (cf. Houtman and Speed, 1983). A measure of stratum information about the contrasts is efficiency factors calculated as eigenvalues of information matrices for the treatment combinations, $\boldsymbol{A}_f$, f = 1, 2, 3, 4, 5, with respect to $\mathbf{r}^{-\delta}$ (e.g. Ambroży and Mejza, 2002), where $\mathbf{r}^{-\delta} = \mathrm{diag}(1/r_1, 1/r_2, \ldots, 1/r_v)$, and r_i denotes the number of replicates of the i-th treatment combination.

3. Method of construction of resolvable SBP designs

We now introduce the semi-Kronecker product of matrices that will be used with this construction procedure (Khatri and Rao, 1968; Rao and Mitra, 1971; Mejza et al., 2020). Let

$\boldsymbol{D} = [\boldsymbol{D}_1 \vdots \boldsymbol{D}_2 \vdots \cdots \vdots \boldsymbol{D}_d]$, $\boldsymbol{E} = [\boldsymbol{E}_1 \vdots \boldsymbol{E}_2 \vdots \cdots \vdots \boldsymbol{E}_d]$, $\boldsymbol{F} = [\boldsymbol{F}_1 \vdots \boldsymbol{F}_2 \vdots \cdots \vdots \boldsymbol{F}_d]$

be three partitioned matrices with the same number of partitions (equal to *d*). The semi-Kronecker product is

$$\mathbf{D} \widetilde{\otimes} \mathbf{E} \widetilde{\otimes} \mathbf{F} = [\mathbf{D}_1 \otimes \mathbf{E}_1 \otimes \mathbf{F}_1 \vdots \mathbf{D}_2 \otimes \mathbf{E}_2 \otimes \mathbf{F}_2 \vdots \cdots \vdots \mathbf{D}_d \otimes \mathbf{E}_d \otimes \mathbf{F}_d], \qquad (3.1)$$

where $\otimes$ denotes the usual Kronecker product of matrices.

Let $\mathbf{N}_A$, $\mathbf{N}_B$, $\mathbf{N}_C$ be incidence matrices of so-called generating subdesigns for the factors *A*, *B* and *C*, respectively. In this construction the matrix $\mathbf{N}_A = \mathbf{1}_s \mathbf{1}_r'$ is the incidence matrix of a randomized complete block design (RCB).

Then let $\mathbf{N}_B = [\mathbf{N}_{B1} \vdots \mathbf{N}_{B2} \vdots \cdots \vdots \mathbf{N}_{B\mathrm{r}}]$ and $\mathbf{N}_C = [\mathbf{N}_{C1} \vdots \mathbf{N}_{C2} \vdots \cdots \vdots \mathbf{N}_{C\mathrm{r}}]$ be the incidence matrices of two square lattice designs SLD(s_1^2, r, s_1) and SLD(s_2^2, r, s_2) with the same number of replicates *r*, where $\mathbf{N}_{Bi}$ and $\mathbf{N}_{Ci}$ correspond to these replicates with s_1 $(= k_2)$ and s_2 $(= k_3)$ plots per block in the columns and subplots within each whole plots, respectively, and $s_1^2 = t$ and $s_2^2 = w$ denote the number of *B* treatments and *C* treatments, respectively. In the SBP considered we can express the incidence matrix $\mathbf{N}_1$ as

$$\boldsymbol{N}_1 = \boldsymbol{N}_A \widetilde{\otimes} \boldsymbol{N}_B \widetilde{\otimes} \boldsymbol{N}_C =$$
$$= [\mathbf{1}_s \otimes \boldsymbol{N}_{B1} \otimes \boldsymbol{N}_{C1} \vdots \mathbf{1}_s \otimes \boldsymbol{N}_{B2} \otimes \boldsymbol{N}_{C2} \vdots \cdots \vdots \mathbf{1}_s \otimes \boldsymbol{N}_{Br} \otimes \boldsymbol{N}_{Cr}] \qquad (3.2)$$

Since the general forms of other incidence matrices $\mathbf{N}_2$ (with respect to the rows), $\mathbf{N}_3$ (with respect to the columns) and $\mathbf{N}_4$ (with respect to the whole plots) are not unique, we present concurrence matrices $\mathbf{N}_2\mathbf{N}_2'$, $\mathbf{N}_3\mathbf{N}_3'$ and $\mathbf{N}_4\mathbf{N}_4'$:

$$\boldsymbol{N}_2\boldsymbol{N}_2' = \sum_{i=1}^{r} (\boldsymbol{I}_s \otimes (\boldsymbol{N}_{Bi}\boldsymbol{N}_{Bi}') \otimes (\boldsymbol{N}_{Ci}\boldsymbol{N}_{Ci}')) \qquad (3.3)$$
$$\boldsymbol{N}_3\boldsymbol{N}_3' = \sum_{i=1}^{r} (\mathbf{1}_s\mathbf{1}_s' \otimes \boldsymbol{I}_{s_1^2} \otimes (\boldsymbol{N}_{Ci}\boldsymbol{N}_{Ci}'))$$
$$\boldsymbol{N}_4\boldsymbol{N}_4' = \sum_{i=1}^{r} (\boldsymbol{I}_s \otimes \boldsymbol{I}_{s_1^2} \otimes (\boldsymbol{N}_{Ci}\boldsymbol{N}_{Ci}')).$$

In this method the number of the treatment combinations is equal to $v = stw = ss_1^2s_2^2$, the number of blocks is $b = rs_1s_2$, and the number of all units is $n = bk_1k_2k_3 = rss_1^2s_2^2$.

As mentioned above, the statistical properties of the incomplete SBP design relate mainly to algebraic properties of the stratum information matrices $\mathbf{A}_f$, $f = 1, \ldots, 5$. These matrices are:

$$\mathbf{A}_0 = \frac{r}{v}\mathbf{J}_v, \quad \mathbf{A}_1 = \frac{1}{ss_1s_2}\mathbf{N}_1\mathbf{N}_1' - \frac{r}{v}\mathbf{J}_v, \quad \mathbf{A}_2 = \frac{1}{s_1s_2}\mathbf{N}_2\mathbf{N}_2' - \frac{1}{ss_1s_2}\mathbf{N}_1\mathbf{N}_1' \tag{3.4}$$

$$\boldsymbol{A}_3 = \frac{1}{ss_2}\boldsymbol{N}_3\boldsymbol{N}_3' - \frac{1}{ss_1s_2}\boldsymbol{N}_1\boldsymbol{N}_1',$$

$$\boldsymbol{A}_4 = \frac{1}{ss_1s_2}\boldsymbol{N}_1\boldsymbol{N}_1' + \frac{1}{s_2}\boldsymbol{N}_4\boldsymbol{N}_4' - \frac{1}{s_1s_2}\boldsymbol{N}_2\boldsymbol{N}_2' - \frac{1}{ss_2}\boldsymbol{N}_3\boldsymbol{N}_3'$$

$$\boldsymbol{A}_5 = r\boldsymbol{I}_v - \frac{1}{s_2}\boldsymbol{N}_4\boldsymbol{N}_4'$$

On analyzing the algebraic properties of the matrices (3.4), we obtain information about the estimability of the treatment contrasts in the strata and their stratum efficiency factors (Table 1).

Table 1. Stratum efficiency factors of the SBP design (by semi-Kronecker product of matrices)

Type of contrasts	Df	strata				
		(1)	(2)	(3)	(4)	(5)
A	$s-1$	–	1	–	–	–
B	$r(s_1-1)$	1/ *r*	–	1 – 1/*r*	–	–
C	$r(s_2-1)$	1/ *r*	–	–	–	1 – 1/*r*
	$s_2^2 - r(s_2-1) - 1$	–	–	–	–	1
A×*B*	$(s-1)r(s_1-1)$	–	1/ *r*	–	1 – 1/*r*	–
A×*C*	$(s-1)r(s_2-1)$	–	1/ *r*	–	–	1 – 1/*r*
	$(s-1)[s_2^2 - r(s_2-1) - 1]$	–	–	–	–	1
B×*C*	$r(s_1-1)(s_2-1)$	1/ *r*	–	–	–	1 – 1/*r*
	$r(\mathrm{r}-1)(s_1-1)(s_2-1)$	–	–	1/ *r*	–	1 – 1/*r*
	$r(s_1-1)[s_2^2 - r(s_2-1) - 1]$	–	–	–	–	1
A×*B*×*C*	$(s-1)r(s_1-1)(s_2-1)$	–	1/ *r*	–	–	1 – 1/*r*
	$(s-1)r(\mathrm{r}-1)(s_1-1)(s_2-1)$	–	–	–	1/ *r*	1 – 1/*r*
	$(s-1)r(s_1-1)[s_2^2 - r(s_2-1) - 1]$	–	–	–	–	1

(1) – the inter-block stratum, (2) – the inter-row stratum, (3) – the inter-column stratum, (4) – the inter-whole plot stratum, (5) – the inter-subplot stratum

4. Example

To illustrate the theory presented in this paper, consider a $(2 \times 4 \times 9)$ - experiment of SBP type. The *A* treatments ($s = 2$) are allocated on two rows as in a complete SBP design, whereas the *B* treatments ($s_1^2 = 4$) and the *C* treatments ($s_2^2 = 6$) are allocated in different square lattice designs with the incidence matrices $\mathbf{N}_B = [\mathbf{N}_{B1} \vdots \mathbf{N}_{B2} \vdots \cdots \vdots \mathbf{N}_{Br}]$ $(\mathrm{SLD}(s_1^2, r, s_1))$ and $\mathbf{N}_C = [\mathbf{N}_{C1} \vdots \mathbf{N}_{C2} \vdots \cdots \vdots \mathbf{N}_{Cr}]$ $(\mathrm{SLD}(s_2^2, r, s_2))$, respectively. Assume that these incidence matrices have the following form (see Clatworthy, 1973):

$$\boldsymbol{N}_B = \begin{bmatrix} 1 & 0 \vdots 1 & 0 \vdots 1 & 0 \\ 1 & 0 \vdots 0 & 1 \vdots 0 & 1 \\ 0 & 1 \vdots 1 & 0 \vdots 0 & 1 \\ 0 & 1 \vdots 0 & 1 \vdots 1 & 0 \end{bmatrix}$$

$$\boldsymbol{N}_C = \begin{bmatrix} 1 & 0 & 0 \vdots 1 & 0 & 0 \vdots 1 & 0 & 0 \\ 1 & 0 & 0 \vdots 0 & 1 & 0 \vdots 0 & 1 & 0 \\ 1 & 0 & 0 \vdots 0 & 0 & 1 \vdots 0 & 0 & 1 \\ 0 & 1 & 0 \vdots 1 & 0 & 0 \vdots 0 & 0 & 1 \\ 0 & 1 & 0 \vdots 0 & 1 & 0 \vdots 1 & 0 & 0 \\ 0 & 1 & 0 \vdots 0 & 0 & 1 \vdots 0 & 1 & 0 \\ 0 & 0 & 1 \vdots 1 & 0 & 0 \vdots 0 & 1 & 0 \\ 0 & 0 & 1 \vdots 0 & 1 & 0 \vdots 0 & 0 & 1 \\ 0 & 0 & 1 \vdots 0 & 0 & 1 \vdots 1 & 0 & 0 \end{bmatrix}.$$

with 3 replicates. Using the semi-Kronecker product $\mathbf{N}_1 = \mathbf{N}_A \widetilde{\otimes} \mathbf{N}_B \widetilde{\otimes} \mathbf{N}_C$ (see 3.2) we obtain the incomplete SBP design with parameters: $v = 72$, $b = 18$, $k = 12$, $\mathbf{r} = 3\mathbf{1}_{72}$, $n = 216$. If we had used $\otimes$ in the construction procedure we would have obtained $b = 54$ blocks with $n = 648$ experimental units.

Note that the proposed final design uses only 33% of the units that would have been required if the same method had been used but based on the usual Kronecker product. Of course, in this last design, all contrasts would be estimated with full efficiency. Usually, in experimental research, some treatment contrasts are more important, and we want to estimate them with higher precision. Some of the less important ones can be estimated with less efficiency.

The effectiveness of treatment contrasts is related to the eigenvalue of the information matrix and the corresponding eigenvector. The eigenvalues of the information matrix of the proposed design are multiple. This means that we have some freedom in choosing the structure of eigenvectors. In this way, we can take into account partially or even completely the researcher's suggestions regarding the ranking of the treatment contrasts by importance. Some of the object contrasts are estimable with full efficiency. These are especially interesting, and it is worth becoming acquainted with the structure (meaning) of the treatment contrasts.

The efficiency factors of the SBP design in strata with respect to the contrasts are given in Table 2.

Table 2. Stratum efficiency factors of the SBP design in this example

Type of contrast	Df	Strata				
		(1)	(2)	(3)	(4)	(5)
A	1	–	1	–	–	–
B	3	1/ 3	–	2 /3	–	–
C	6	1/ 3	–	–	–	2 /3
	2	–	–	–	–	1
$A\times B$	3	–	1/ 3	–	2 /3	–
$A\times C$	6	–	1/ 3	–	–	2 /3
	2	–	–	–	–	1
$B\times C$	6	1/ 3	–	–	–	2 /3
	12	–	–	1/ 3	–	2 /3
	6	–	–	–	–	1
$A\times B\times C$	6	–	1/ 3	–	–	2 /3
	12	–	–	–	1/ 3	2 /3
	6	–	–	–	–	1

All notations in Table 2 are the same as in Table 1.

It may be observed that using the incomplete SBP design from the example, contrasts among A treatments are estimated in the stratum (2) with full efficiency (=1) as in a complete SBP design. The remaining contrasts are estimated in two

strata with stratum efficiencies of 1/3 and 2/3, or in one stratum with full efficiency.

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