ON THE EFFICIENCY OF ORTHOGONAL TREATMENT
CONTRASTS IN MULTISTRATUM INCOMPLETE SPLIT-SPLIT-PLOT DESIGNS CONSTRUCTED BY SQUARE LATTICE DESIGNS

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Summary

We construct an incomplete split-split-plot design for three factor experiments. The method is based on a semi-Kronecker (Khatri-Rao) product of three matrices. We use two square lattice designs for whole plot treatments and subplot treatments and also a randomized complete block design for sub-subplot treatments. So in the paper we consider a situation when the split-split-plot design is incomplete with respect to two factors. The considered design is characterized with respect to general balance property. We give stratum efficiency factors useful in planning incomplete experimental designs and in the statistical analysis.

Key words and phrases: square lattice design, general balance, incomplete split-split-plot design, Khatri-Rao product of matrices, stratum efficiency factors.

Classification AMS 2010: 62K10, 62K15

1. Introduction

Incomplete split-split-plot (shortly, SSP) designs are an alternative for orthogonal (complete) SSP designs which are usually used for three or more factor
experiments. In both cases the experimental blocks should have suitable structure with nested units (whole plots, subplots and sub-subplots). A number of them is related to the applied method of a construction of the design and desirable statistical properties. Additionally, the SSP design is required to satisfy one of the most important principles in the theory of block designs – homogeneity of units within given block structure, the whole plot structure and the subplot structure. Planned incompleteness of the SSP design is one of the ways to overcome difficulties when the number of the suitable units is insufficient to allocate the whole plot treatments or/and subplot treatments or/and sub-subplot treatments inside the blocks.

We consider the incomplete SSP designs with orthogonal block structure only (Nelder, 1965a, 1965b). Modeling and analysis of data obtained from such experiments were presented, for instance, in Mejza I. (1997a, 1997b). Additionally, some characterization of the incomplete SSP designs may be found in Ambroży and Mejza (2011, 2013), Ambroży-Deręgowska and Mejza (2014, 2015). Authors have mainly considered construction of the SSP designs for which the incidence matrix with respect to blocks is Kronecker product of incidence matrices for subdesigns (efficiency or partial efficiency balanced designs). The SSP designs obtained by this way usually have a large number of units, which is sometimes unprofitable situation (e.g. because of a cost of an experiment).

In the present paper we consider a construction procedure of an incomplete SSP design based on a semi-Kronecker product called also Khatri-Rao product of matrices. This method leads to new designs with the number of units less than the number of units obtained by using the usual Kronecker product. Square Lattice Designs (shortly, SLDs), (see e.g. Raghavarao, 1971; Caliński and Kageyama, 2003) for the whole plot treatments and for the subplot treatments are used to construct new SSP designs. The statistical properties, such general balance and stratum balance (e.g. Houtman and Speed, 1983; Mejza S., 1992) of the final designs are examined in the paper, see (4.6). Planning and an analysis of data obtained from such experiments can be performed using efficiency factors presented in the present paper.

2. Material structure

Let us take a three-factor experiment of an incomplete SSP type 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 $C_1, C_2, \ldots, C_w$. Thus the number $v = stw$ denotes the number of all treatment combinations in the experiment.
There is assumed the experimental material can be divided into $b$ blocks with $k_1$ whole plots. We assume also, that the blocks can be grouped into $r$ replicates (superblocks, resolution classes). Then, each whole plot inside the blocks is divided into $k_2$ subplots with $k_3$ sub-subplots. The $s$ ($s > k_1$) levels of factor $A$ (whole plot treatments) are randomly allotted to the whole plots within each block, $t$ ($t > k_2$) levels of factor $B$ (subplot treatments) are randomly allotted to the subplots within each whole plot, and the $w$ ($w = k_3$) levels of factor $C$ (sub-subplot treatments) are randomly allotted to the sub-subplots within each subplot.

In the paper it is assumed the SSP design is incomplete with respect to the levels of the factors $A$ and $B$, and complete with respect to the levels of the factor $C$ ($k_1 < s$, $k_2 < t$, $k_3 = w$), i.e. not all $v$ treatment combinations are inside each block. The decision which of them occur in the blocks is based on the construction method given in Section 4.

3. Linear model

As a result of certain assumptions and performed four randomization processes in the experiment the mixed linear model of vector $y$ of $n = bk_1k_2k_3$ observations has the form:

$$ y = \Delta'\tau + \sum_{f=1}^{4} D_f \eta_f + e, \tag{3.1} $$

and the following properties:

$$ E(y) = \Delta'\tau, \quad \text{Cov}(y) = \mathbf{V}(\gamma) \tag{3.2} $$

where $\Delta'$ is a known design matrix for $v = stw$ treatment combinations, $\tau$ ($v \times 1$) is the vector of fixed treatment combination parameters, $D_1', D_2', D_3', D_4'$ are respectively, $(n \times b)$, $(n \times bk_1)$, $(n \times bk_1k_2)$, $(n \times bk_1k_2k_3)$ - design matrices for blocks, the whole plots (within the blocks), the subplots (within the whole plots inside the blocks), and the sub-subplots (within the subplots inside the whole plots and blocks).

The $\eta_f$ ($f = 1, 2, 3, 4$) are, respectively, random effect vectors of the blocks, the whole plots, the subplots, the sub-subplots.
According to the assumed orthogonal block structure of the considered SSP design, the covariance matrix (3.2) can be written as $\text{Cov}(\mathbf{y}) = \sum_{f=0}^{4} \gamma_f \mathbf{P}_f$, where $\mathbf{P}_f$ are a family of known pairwise orthogonal projection operators (projectors) summing to the identity matrix (cf. Houtman and Speed, 1983). The range space $\mathfrak{R}\{\mathbf{P}_f\}$ of $\mathbf{P}_f$, $f = 0, 1, \ldots, 4$, is termed the $f$-th stratum of the model, and $\{\gamma_f\}$ are unknown strata variances. So this model can be analysed using the methods based on Nelder’s approach to the multistratum experiments (Nelder, 1965a, 1965b). In the SSP model there are five strata, i.e. the total area stratum (zero stratum), the inter-block stratum (the first stratum), the inter-whole plot stratum (the second stratum), the inter-subplot stratum (the third stratum) and the inter-sub-subplot stratum (the fourth stratum).

The considered SSP design will be characterized with respect to stratum efficiencies for chosen groups of contrasts among treatment combination parameters with regard to general balance property (cf. Houtman and Speed, 1983, Mejza S., 1992). A measure of stratum information about the contrasts is defined as eigenvalues of information matrices for the treatment combinations, $\mathbf{A}_f$, $f = 1, 2, 3, 4$, with respect to $\mathbf{r}^{-5}$, where $\mathbf{r}^{-5} = \text{diag}(1/r_1, 1/r_2, \ldots, 1/r_v)$, and $r_i$ ($i = 1, 2, \ldots, v$) denote replications of the $v$ treatment combinations.

**4. Method of construction**

Now we introduce the semi-Kronecker product of three matrices (see, Khatri and Rao, 1968, Rao and Mitra, 1971, Ambroży and Mejza, 2003) that will be used to construct the incomplete SSP design.

Let

$$
\mathbf{D} = [\mathbf{D}_1 : \mathbf{D}_2 : \cdots : \mathbf{D}_r], \quad \mathbf{E} = [\mathbf{E}_1 : \mathbf{E}_2 : \cdots : \mathbf{E}_r], \quad \mathbf{F} = [\mathbf{F}_1 : \mathbf{F}_2 : \cdots : \mathbf{F}_r]
$$

be three partitioned matrices with the same number of partitions (equal to $r$).

**Definition.** The semi-Kronecker product of three matrices $\mathbf{D}$, $\mathbf{E}$, $\mathbf{F}$ given above will be as follows:

$$
\mathbf{D} \boxtimes \mathbf{E} \boxtimes \mathbf{F} = [\mathbf{D}_1 \boxtimes \mathbf{E}_1 \boxtimes \mathbf{F}_1 : \mathbf{D}_2 \boxtimes \mathbf{E}_2 \boxtimes \mathbf{F}_2 : \cdots : \mathbf{D}_r \boxtimes \mathbf{E}_r \boxtimes \mathbf{F}_r],
$$
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where \( \otimes \) denotes the usual Kronecker product of two matrices.

Let \( \mathbf{N}_A, \mathbf{N}_B \) be incidence matrices of so called generating subdesigns for the factors \( \mathbf{A} \) and \( \mathbf{B} \), respectively. In this construction the matrices

\[
\mathbf{N}_A = \left[ \mathbf{N}_{A_1} : \mathbf{N}_{A_2} : \cdots : \mathbf{N}_{A_r} \right] \quad \text{and} \quad \mathbf{N}_B = \left[ \mathbf{N}_{B_1} : \mathbf{N}_{B_2} : \cdots : \mathbf{N}_{B_r} \right] \quad (4.1)
\]

are the incidence matrices of square lattice designs (SLD), (e.g. Raghavarao, 1971): SLD\( (a_1^2, r, a_1) \) and SLD\( (a_2^2, r, a_2) \) with the same number of replicates \( r \), where \( \mathbf{N}_{A_i} (a_1^2 \times a_1) \) and \( \mathbf{N}_{B_i} (a_2^2 \times a_2) \) correspond to these replicates with \( a_1 = k_1 \) and \( a_2 = k_2 \) plots per block (i.e. the whole plots inside each block and the subplots inside each whole plot in the SSP design, respectively), and \( a_1^2 = s \) and \( a_2^2 = t \) denote the number of \( \mathbf{A} \) treatments and \( \mathbf{B} \) treatments while \( r \leq a_1 + 1, r \leq a_2 + 1 \) respectively.

While \( \mathbf{N}_C = \mathbf{1}_w \mathbf{1}'_r \) is an incidence matrix of a randomized complete block (RBD) design (for the factor \( \mathbf{C} \)).

It is known generally the SLDs are resolvable designs such that for any pair of different superblocks, any block of one of them and any block of another superblock contain just one common treatment. From this fact we obtain some relations

\[
\mathbf{N}'_{A_i} \mathbf{N}_{A_i} = a_1 \mathbf{I}_{a_1}, \quad \mathbf{N}'_{B_i} \mathbf{N}_{B_i} = a_2 \mathbf{I}_{a_2}, \quad \mathbf{N}'_{A_i} \mathbf{N}_{B_i} = \mathbf{1}_{a_1} \mathbf{1}'_{a_2}, \quad (4.2)
\]

where \( i, j = 1, 2, \ldots, r, \ i \neq j \).

In the SSP design considered we can express the incidence matrix \( \mathbf{N}_i \) (with respect to the blocks) as

\[
\mathbf{N}_i = \mathbf{N}_A \otimes \mathbf{N}_B \otimes \mathbf{N}_C = \mathbf{N}_A \otimes \mathbf{N}_B \otimes \mathbf{1}_w \mathbf{1}'_r = \\
\left[ \mathbf{N}_{A_1} \otimes \mathbf{N}_{B_1} : \mathbf{N}_{A_2} \otimes \mathbf{N}_{B_2} : \cdots : \mathbf{N}_{A_r} \otimes \mathbf{N}_{B_r} \otimes \mathbf{1}_w \right]. \quad (4.3)
\]

General forms of other incidence matrices \( \mathbf{N}_2 \) (with respect to the whole plots) and \( \mathbf{N}_3 \) (with respect to the subplots) are not unique. However, corresponding to them concurrence matrices \( \mathbf{N}_i \mathbf{N}'_i, \ i = 2, 3, \) are unique (see (4.5)). But if we arrange the whole plots and subplots in suitable orders we can express \( \mathbf{N}_2 \) and \( \mathbf{N}_3 \) as follows

\[
\mathbf{N}_2 = \left[ \mathbf{I}_{a_1^2} \otimes \mathbf{N}_{B_1} \otimes \mathbf{1}_w : \mathbf{I}_{a_1^2} \otimes \mathbf{N}_{B_2} \otimes \mathbf{1}_w : \cdots : \mathbf{I}_{a_1^2} \otimes \mathbf{N}_{B_r} \otimes \mathbf{1}_w \right], \quad (4.4)
\]

In this method of the construction the number of the treatment combinations is equal to \( \nu = stw = a_1^0a_2^2w \), the number of the blocks is \( b = ra_1a_2 \) and the number of all units is \( n = bk_1k_2k_3 = ra_1^2a_2^2w \).

Now, applying (4.3) and (4.4) the concurrence matrices take the forms:

\[
N_iN'_i = \sum_{j=1}^{i}(N_{ij}N'_{ij}) \otimes (N_{ij}N'_{ij}) \otimes 1_{w'}', \\
N_iN'_2 = \sum_{j=1}^{i}(I_{a_1} \otimes (N_{ij}N'_{ij}) \otimes 1_{w'}), \tag{4.5}
\]

\[
N_iN'_3 = \sum_{j=1}^{i}(I_{a_1} \otimes I_{a_2} \otimes 1_{w'}). \\
\]

To obtain stratum efficiency factors we have to check if the incomplete SSP design is generally balanced (cf. Houtman and Speed, 1983, Mejza S., 1992). From (4.2) and (4.5) we can see that the concurrence matrices \( N_iN'_j, i = 1, 2, 3 \), are commutative, i.e.

\[
N_iN'_j = N_jN'_i, \tag{4.6}
\]

hold for \( i \neq j, j = 1, 2, 3 \).

From (4.6) we can obtain that considered SSP designs are generally balanced. From this fact results the information matrices \( A_f, f = 1, 2, 3, 4 \), have the same set of eigenvectors (with respect to \( r^{\delta} \)) defining the orthogonal (basic) contrasts. Hence, if a group of the same contrasts is estimable in two or more different strata, we have two possibilities. We can perform a statistical analysis of these contrasts in each stratum separately only or combine the obtained information on these contrasts from the relevant strata (see e.g., Caliński and Kageyama, 2000).

However, each of these methods involves loss of information in the estimation and detailed testing associated with these contrasts. You can limit this loss, for example, if the contrasts of experimental interest are estimated with full efficiency (as in the proposed construction method), see Table 1.

Finally, the matrices \( A_f \) are the following:

\[
A_0 = \frac{r}{\nu} J, \quad A_1 = \frac{1}{a_1a_2w} N_iN'_i - \frac{r}{\nu} J, \quad A_2 = \frac{1}{a_2w} N_iN'_2 - \frac{1}{a_1a_2w} N_iN'_1.
\]
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\[
A_i = \frac{1}{w} N_iN_i' - \frac{1}{a_i w} N_iN_i' \quad A_i = rI_i - \frac{1}{w} N_iN_i'.
\] (4.7)

Eigenvalues of the matrices (4.7) with respect the replicates, called stratum efficiency factors of the SSP design, corresponding to the orthogonal contrasts are given in Table 1.

<table>
<thead>
<tr>
<th>Type of contrast</th>
<th>df</th>
<th>Strata</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>I</td>
<td>II</td>
</tr>
<tr>
<td>A</td>
<td>1/r</td>
<td>1 - 1/r</td>
</tr>
<tr>
<td>B</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>C</td>
<td>1/r</td>
<td>–</td>
</tr>
<tr>
<td>AxB</td>
<td>1/r</td>
<td>–</td>
</tr>
<tr>
<td>AxC</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>BxC</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>AxBxC</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

I – the inter-block stratum, II – the inter-whole plot stratum, III – the inter-subplot stratum, IV – the inter-sub-subplot stratum

5. Example and discussion

To illustrate the theory presented in the paper, consider a \((4 \times 9 \times 2)\) - experiment arranged in the incomplete SSP design. The \(A\) treatments and the \(B\) treatments are allocated in the different balanced lattice designs with the incidence matrices \(N_A = \left[N_A^T : N_A^T : N_A^T \right] (\text{SLD}(4, \ 3, \ 2))\) and \(N_B = \left[N_B^T : N_B^T : N_B^T \right] (\text{SLD}(9, \ 3, \ 3))\), respectively. Assume that these incidence matrices have the following forms (see Clatworthy, 1973):
The treatments occur in a randomized complete block design. Then the incidence matrix \( N_i \) of the incomplete SSP design as follows

\[
N_i = N_A \otimes N_B \otimes 1_N^1.
\]

To present a sample layout of the considered SSP design we introduce an abbreviation.

Let \( \{A_i, A_j | B_l, B_m, B_p | C_1, C_2 \} \) denotes a block such that \( A_i, A_j \), where \( i, j \in \{1, 2, 3, 4\}, i \neq j \), are the whole plot treatments inside the block, \( B_l, B_m, B_p \), where \( l, m, p \in \{1, 2, 3, 4, 5, 6, 7, 8, 9\}, l \neq m \neq p \), are the subplot treatments in each whole plot and \( C_1, C_2 \) are the sub-subplot treatments in each subplot inside the block.

Then the incomplete SSP design can be expressed by the following way:

\[
\begin{align*}
\{A_1, A_2 | B_1, B_2, B_3 | C_1, C_2 \}, & \quad \{A_1, A_2 | B_4, B_5, B_6 | C_1, C_2 \}, \\
\{A_1, A_2 | B_7, B_8, B_9 | C_1, C_2 \}, & \quad \{A_3, A_4 | B_1, B_2, B_3 | C_1, C_2 \}, \\
\{A_3, A_4 | B_4, B_5, B_6 | C_1, C_2 \}, & \quad \{A_3, A_4 | B_7, B_8, B_9 | C_1, C_2 \}, \\
\{A_1, A_3 | B_1, B_4, B_7 | C_1, C_2 \}, & \quad \{A_1, A_3 | B_2, B_5, B_8 | C_1, C_2 \}, \\
\{A_1, A_3 | B_3, B_6, B_9 | C_1, C_2 \}, & \quad \{A_2, A_4 | B_1, B_4, B_7 | C_1, C_2 \}, \\
\{A_2, A_4 | B_2, B_5, B_8 | C_1, C_2 \}, & \quad \{A_2, A_4 | B_3, B_6, B_9 | C_1, C_2 \}, \\
\{A_1, A_4 | B_1, B_5, B_9 | C_1, C_2 \}, & \quad \{A_1, A_4 | B_2, B_6, B_7 | C_1, C_2 \}.
\end{align*}
\]
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\[ \{A_1, A_4 \mid B_3, B_4, B_8 \mid C_1, C_2\}, \quad \{A_2, A_3 \mid B_1, B_5, B_9 \mid C_1, C_2\}, \]

\[ \{A_2, A_3 \mid B_2, B_6, B_7 \mid C_1, C_2\}, \quad \{A_2, A_3 \mid B_3, B_4, B_8 \mid C_1, C_2\}, \]

Below we show an example of a single block from a sample layout (after three step randomization).

\[
\begin{array}{c|c|c|c|c|c|c}
B_2 & A_2 & B_3 & A_1 & B_1 & B_3 & B_2 \\
C_2 & C_1 & C_2 & C_1 & C_1 & C_2 & C_1
\end{array}
\]

**Fig. 1.** Random assignment of the levels of three factors in one block of the SSP design.

Note that using the proposed construction method, the resulting SSP design has \( b = 18 \) blocks with size equal to 12 (two whole plots, three subplots and two sub-subplots). So, the parameters of the final incomplete SSP design are equal to \( v = 72, \ b = 18, \ k = 12, \ r = 31, n = 216. \)

If we had used \( \otimes \) in the construction procedure we would have obtained \( b = r^2a_1a_2 = 54 \) blocks with \( n = 648 \) experimental units. Generally, the number of blocks of the design obtained by usual Kronecker product is \( t \) times larger than those of the design obtained by the semi-Kronecker product.

Then notice that Table 2 indicates the stratum efficiency factors of the incomplete SSP design and the numbers of the orthogonal contrasts which are estimable in suitable for them strata (see Table 1). The orthogonal contrasts can be built using, for example, the method presented in the paper of Ambroży-Deregowska and Mejza (2015).

It is worth noticing that in the presented incomplete SSP design two contrasts among \( B \) treatments and six interaction contrasts of type \( A \times B \) are estimated with full efficiency (equal to 1) in the inter-subplot stratum (III). It results from the utilized construction method.

The remaining contrasts of types \( B \) and \( A \times B \) are estimated with not full efficiency in two strata: I – the inter-block stratum or II – the inter-whole plot stratum and in the inter-subplot stratum (III). Also information about the contrasts among \( A \) treatments is included in two strata (about 33% in the inter-block stratum and 67% in the inter-whole plot stratum). The remaining contrasts among \( C \) treatments and all interaction contrasts related to this factor are estimated with full efficiency in appropriate for them strata as in a complete SSP design.
Table 2. Stratum efficiency factors of the example SSP design

<table>
<thead>
<tr>
<th>Type of contrast</th>
<th>df</th>
<th>Strata</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>I</td>
</tr>
<tr>
<td>A</td>
<td>3</td>
<td>1/3</td>
</tr>
<tr>
<td>B</td>
<td>2</td>
<td>–</td>
</tr>
<tr>
<td>C</td>
<td>6</td>
<td>1/3</td>
</tr>
<tr>
<td>A×B</td>
<td>12</td>
<td>–</td>
</tr>
<tr>
<td>A×C</td>
<td>6</td>
<td>–</td>
</tr>
<tr>
<td>B×C</td>
<td>8</td>
<td>–</td>
</tr>
<tr>
<td>A×B×C</td>
<td>24</td>
<td>–</td>
</tr>
</tbody>
</table>

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

As we mentioned earlier, in the cases of the contrasts that are estimated with different efficiencies in two strata of the experiment, one can try to recover the inter-block stratum information using one of the information recovery methods. Methods dealing with this problem are known in the literature (see, e.g. Caliński and Kageyama, 2000).

Note, however, that most, nearly 67% of information about certain contrasts of type A, B and A×B occurs in the II and III strata. It seems it is sufficient to carry out particular analyses related to those contrasts. Each of them gives the best linear unbiased estimator in the relevant strata.

In addition, note that all A, B and A×B type contrasts are estimated with full or not full efficiency in the inter-whole plot stratum (II) or the inter-subplot stratum (III), respectively. In such case one can test the general hypotheses related to these sources of variation in these strata.

References

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