Listy Biometryczne - Biometrical Letters
Vol. 35(1998), No. 2, 107-115

On properties and models in the block design theory*

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SUMMARY

The theory of block designs is composed of some general ideas, various properties, and different models. In this note we show interrelations between them indicating, in particular, their sensibility and usefulness in specific experimental situations. We start from the most classic fixed model, which seems to be the main source of the whole theory, and end with mixed randomized models, which were widely discussed by Professor Tadeusz Caliński through the last decade.

KEY WORDS: connectedness, estimability, best linear unbiased estimator, variance balance, randomization

1. Introduction and preliminaries

The main concept of the block design theory is, of course, a block. It is a collection of some units forming a base for comparing the treatments. In the case of field experiments, the units are plots and the treatments are varieties, fertilizers, growing conditions etc. To make the comparisons precise, the plots in blocks should be homogeneous. In the most ideal situation, all plots of each block should be identical with respect to the size, natural fertility, shading, natural soil humidity etc. The plots from different blocks can differ. Having such blocks, the experimenter applies chosen treatments on the plots. Each plot receives one treatment, and produces one observation.

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*The paper was submitted on the occasion of 70-th birthday of Professor Tadeusz Caliński.

The vector $\mathbf{y}$ of all observations, obtained from a block design experiment with identical plots in each block, can be modeled by the equation

$$\mathbf{y} = \mathbf{1}\mu + \mathbf{\Delta}'\boldsymbol{\tau} + \mathbf{D}'\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \tag{1}$$

where μ is an unknown parameter common to all n measurements, $\boldsymbol{\tau}$ is a v-vector of unknown treatment effects, $\boldsymbol{\beta}$ is a b-vector of unknown block effects, $\boldsymbol{\varepsilon}$ is a standard n-vector of random errors, while $\mathbf{1}$, $\mathbf{\Delta}'$ and $\mathbf{D}'$ are the n-vector of units, the $n \times v$ known design matrix for treatments, and the $n \times b$ design matrix for blocks, respectively.

The relations between blocks and treatments are also uniquely reflected by the $v \times b$ incidence matrix $\mathbf{N}$,

$$\mathbf{N} = \mathbf{\Delta}\mathbf{D}', \tag{2}$$

in which the ij-th element, n_{ij}, is equal to the number of plots in the j-th block receiving the i-th treatment. Summing the columns of $\mathbf{N}$, we obtain the v-vector $\mathbf{r}$ of replications, $\mathbf{N1} = \mathbf{r}$, and summing the rows of $\mathbf{N}$, we obtain the b-vector $\mathbf{k}$ of block sizes, $\mathbf{N}'\mathbf{1} = \mathbf{k}$.

In the statistical analysis of data from the block design, the key role plays the $v \times v$ matrix $\mathbf{C}$. It has the form

$$\mathbf{C} = \mathbf{r}^{\delta} - \mathbf{N}\mathbf{k}^{-\delta}\mathbf{N}', \tag{3}$$

where $\mathbf{r}^{\delta} = \mathbf{\Delta}\mathbf{\Delta}'$ and $\mathbf{k}^{-\delta} = (\mathbf{D}\mathbf{D}')^{-1}$. The matrix $\mathbf{C}$ can also be expressed as

$$\mathbf{C} = \mathbf{\Delta}\boldsymbol{\phi}\mathbf{\Delta}', \tag{4}$$

where

$$\boldsymbol{\phi} = \mathbf{I} - \mathbf{D}'\mathbf{k}^{-\delta}\mathbf{D} \tag{5}$$

is an orthogonal projector, i.e. $\boldsymbol{\phi}^2 = \boldsymbol{\phi} = \boldsymbol{\phi}'$.

2. Connectedness

The main combinatorial property of a block design is its connectedness, as introduced by Bose (1950). This concept can be defined as follows. Two blocks are directly connected if they have a common treatment, and are connected if they can be joined by a chain of directly connected blocks. A block design is connected if all its blocks are connected. The most important result related to this property is as follows.

THEOREM 1. *The block design is connected if and only if* $r(\mathbf{C}) = v - 1$, *where* $r(\mathbf{C})$ *denotes the rank of* $\mathbf{C}$.

Although the definition of connectedness gives the simplest way of verifying this property, Theorem 1 exhibits a direct relation between this combinatorial property and the matrix $\mathbf{C}$ of the design. This property is also simply related with the incidence matrix, defined in (2). If the design is connected, then its incidence matrix $\mathbf{N}$ can not be transformed to a block-diagonal form, by permuting its rows and/or columns. Finally, it should be noted that connectedness is the property which is applicable also beyond the scope of the block design theory.

3. Estimability

The aim of the experiment is to discover the differences between effects of treatments. They can be observed from expected measurements, if it is possible to eliminate the effects of blocks. Let $E(\mathbf{y})$ denote the expectation vector of $\mathbf{y}$. Then, from (1), we have

$$E(\mathbf{y}) = \mathbf{1}\mu + \boldsymbol{\Delta}'\boldsymbol{\tau} + \mathbf{D}'\boldsymbol{\beta}. \tag{6}$$

To eliminate block effects, we can use the orthogonal projector $\boldsymbol{\phi}$ given in (5). Since $\boldsymbol{\phi}\mathbf{D}' = \mathbf{0}$, which implies also $\boldsymbol{\phi}\mathbf{1} = \mathbf{0}$, from (6) we have

$$\boldsymbol{\phi}E(\mathbf{y}) = \boldsymbol{\phi}\boldsymbol{\Delta}'\boldsymbol{\tau}. \tag{7}$$

Since $\boldsymbol{\phi}E(\mathbf{y}) = E(\boldsymbol{\phi}\mathbf{y})$, the equality (7) proves that all functions $\boldsymbol{\phi}\boldsymbol{\Delta}'\boldsymbol{\tau}$ can be estimated unbiasedly by linear transformation of $\mathbf{y}$. This means that functions $\boldsymbol{\phi}\boldsymbol{\Delta}'\boldsymbol{\tau}$ are estimable, which is a statistical property originally introduced by Bose (1944). Moreover, since functions $\boldsymbol{\phi}\boldsymbol{\Delta}'\boldsymbol{\tau}$ depend only on treatment effects, they form the main object of the analysis. The product $\boldsymbol{\phi}\boldsymbol{\Delta}'$ is an $n \times v$ matrix, and it is called the adjusted design matrix for treatments (cf. Caliński and Kageyama, 1996). Therefore, in the set $\boldsymbol{\phi}\boldsymbol{\Delta}'\boldsymbol{\tau}$ we have n estimable functions of treatment effects. Note, moreover, that all of them are contrasts, since $\boldsymbol{\phi}\boldsymbol{\Delta}'\mathbf{1} = \boldsymbol{\phi}\mathbf{1} = \mathbf{0}$. On the other hand observe, that between v objects there are at most $v-1$ linearly independent contrasts. Thus, the set $\boldsymbol{\phi}\boldsymbol{\Delta}'\boldsymbol{\tau}$ can be significantly reduced. It is shown in the following

THEOREM 2. *The function* $\mathbf{p}'\boldsymbol{\tau}$ *of treatment effects is estimable if and only if* $\mathbf{p} \in R(\mathbf{C})$, *where* $R(\mathbf{C})$ *denotes the range of* $\mathbf{C}$.

The most longed situation is, however, characterized by

THEOREM 3. *All treatment contrasts are estimable if and only if* $r(\mathbf{C}) = v - 1$.

Comparing now Theorem 1 with Theorem 3, we can conclude that the block design is connected if and only if all treatment contrasts are estimable. This is the most famous statement of the block design theory, revealing the statistical sense of combinatorial property.

4. Existence of BLUE

From previous discussion we have the following practical conclusion. The estimable functions of treatment parameters are contrasts of the form $\boldsymbol{\phi\Delta'\tau}$ or $\mathbf{C}\boldsymbol{\tau}$. Their unbiased estimators are $\boldsymbol{\phi}\mathbf{y}$ or $\boldsymbol{\Delta\phi}\mathbf{y}$, respectively. But, which is better? The question about the existence and the form of the best linear unbiased estimator (BLUE) of estimable functions is closely related to the dispersion matrix of observations. In our simple model, when the selection of units into blocks is perfect and only standard technical errors are considered, the dispersion matrix of $\mathbf{y}$ is $\sigma^2\mathbf{I}$, where σ^2 is a common error variance. This means that the BLUE of any estimable function can be determined by the least squares method. Therefore, in the context of a simple block design model, we can formulate the following

THEOREM 4. *For each estimable contrast there exists BLUE, which follows from the least square method.*

The least square method is directly connected with the normal equations, which again are related to the matrix $\mathbf{C}$ defined in (3) or (4). Namely, after eliminating block effects, they take the form

$$\mathbf{C}\boldsymbol{\tau}^o = \boldsymbol{\Delta\phi}\mathbf{y}, \tag{8}$$

where $\boldsymbol{\tau}^o$ is the least squares estimate of $\boldsymbol{\tau}$. Thus we can say that the BLUEs of $\mathbf{C}\boldsymbol{\tau}$ contrasts, corresponding to the left hand side of (8), are supplied by their right hand side $\boldsymbol{\Delta\phi}\mathbf{y}$.

The next result establishes one more statistical property of the matrix $\mathbf{C}$. Under the simple block design model, the following holds.

THEOREM 5. *The dispersion matrix of the BLUE of* $\mathbf{C}\boldsymbol{\tau}$ *is proportional to the matrix* $\mathbf{C}$.

So we see, that the best estimation is closely connected with the matrix $\mathbf{C}$. Also the BLUE of $\boldsymbol{\phi\Delta'\tau}$ can be expressed by a solution of (8). It has the form $\boldsymbol{\phi\Delta'}\mathbf{C}^-\boldsymbol{\Delta\phi}\mathbf{y}$, where $\mathbf{C}^-$ is a g-inverse of $\mathbf{C}$.

5. Balance

The balance is a property, which has variety of meanings. It can be related to purely combinatorial features of the blocks as well as with properties of the BLUE. We restrict our discussion only to the variance balance property originated by Vartak (1963) (cf. Caliński and Kageyama, 1996), which has a direct statistical sense. A block design is variance balanced if the BLUE of every estimable treatment contrast $\mathbf{p}'\boldsymbol{\tau}$, such that $\mathbf{p}'\mathbf{p} = 1$, has the same variance. The relation of this concept with the matrix $\mathbf{C}$ reveals the following

THEOREM 6. *The block design is variance balanced if and only if* $\mathbf{C} = \lambda \mathbf{C}^2$.

Under the condition of connectedness, the characterization contained in Theorem 6 gives the equality

$$\mathbf{C} = \lambda\{\mathbf{I} - (1/v)\mathbf{1}\mathbf{1}'\}, \tag{9}$$

which is sometimes considered as a definition of variance balance. This seems an unfortunate approach, since the matrix algebra plays only supporting role both in combinatorial and statistical theory. Note, moreover, that in accordance with the definition, precisely stated by Caliński and Kageyama (1996), the variance balance property has sense only if BLUE of $\mathbf{C}\boldsymbol{\tau}$ exists and Theorem 5 holds.

6. Randomization of plots

The results contained in the previous sections are valid under the simple fixed model. It is justified, if plots in each block are perfectly selected, and thus can be considered as equal. This requirement, however, is never met in field experiments, since the plots are created by nature and the experimenter has a very limited possibility of their selection. In such case, when plots in blocks are not equal, the only remedy is a randomization. If we conduct this process for plots in each block, then we equalize them in probabilistic sense.

After applying treatments to randomly chosen plots, the expectation vector of observations will be the same as in (6). In consequence, the estimability criterion is not changed. The randomization of plots inside the blocks introduces, however, some changes in the structure of the dispersion matrix. It can be expressed (cf. Kala, 1991) as

$$D(\mathbf{y}) = \text{diag}[\sigma^2_{u.j}\{\mathbf{I}_{k_j} - (1/k_j)\mathbf{1}\mathbf{1}'\}] + \sigma^2\mathbf{I}, \tag{10}$$

where k_j is the size of the j-th block, while $\sigma^2_{u.j}$ is the variance of plots forming the j-th block. As we see, there are b extra variance components in the new, more realistic model. Each component characterizes one separate block and reflects the differences which were not eliminated while selecting plots into blocks. The relations between these components are very important from the statistical point of view. If they are different, there is no BLUE for the set of all estimable treatment contrasts $\mathbf{C}\boldsymbol{\tau}$. However, we can estimate them by $\boldsymbol{\Delta\phi}\mathbf{y}$, i.e. by the least squares method, which ensures at least unbiasedness. If the variance components $\sigma^2_{u.j}$, $j = 1, 2, ..., b$, are all equal, i.e. if

$$\sigma^2_{u.1} = \sigma^2_{u.2} = \dots = \sigma^2_{u.b} = \sigma^2_u, \tag{11}$$

then (10) reduces to the form

$$D(\mathbf{y}) = \sigma^2_u \boldsymbol{\phi} + \sigma^2 \mathbf{I}. \tag{12}$$

In consequence, the BLUE of $\mathbf{C}\boldsymbol{\tau}$ exists. It is again the least squares estimator $\boldsymbol{\Delta\phi}\mathbf{y}$. Moreover, its dispersion matrix will be proportional to the matrix $\mathbf{C}$, as in Theorem 5, which preserves the sense of variance balance property. Thus, the homogeneity of variances $\sigma^2_{u.j}$, $j = 1, 2, ..., b$, expressed by the condition (11), does not change the estimation procedure, but it decides about statistical properties of the least squares estimates.

7. Complete randomization

Randomization of plots inside the blocks introduces some comfort in preparing the plots. The experimenter is not forced anymore to select identical plots to each block. The plots in blocks can vary. However, he should worry about their homogeneous spread over all blocks. If the variances of plots from different blocks are comparable, the optimal properties of the least squares estimates are preserved. If not, they are lost. In the latter case, the randomization of blocks is usually proposed (cf. Nelder, 1954, White, 1975, Caliński and Kageyama, 1988, 1991). It is quite radical procedure, since such randomization statistically equalizes whole blocks. It means that the individual effects of blocks disappear from the expectation. Now, it takes the form

$$E(\mathbf{y}) = \mathbf{1}\mu + \boldsymbol{\Delta}'\boldsymbol{\tau}. \tag{13}$$

In such case, all contrasts are estimable, disregarding the connectedness of the design. Therefore, Theorem 2 is not valid. The set of these contrasts can be expressed as $\boldsymbol{\phi}_0\boldsymbol{\Delta}'\boldsymbol{\tau}$, where

$$\boldsymbol{\phi}_0 = \mathbf{I} - (1/n)\mathbf{1}\mathbf{1}' \tag{14}$$

is an orthogonal projector eliminating μ from the expectation (13), or, in the reduced form, as $\mathbf{C}_0\boldsymbol{\tau}$, where $\mathbf{C}_0 = \boldsymbol{\Delta\phi}_0\boldsymbol{\Delta}'$. Their least squares estimator is $\boldsymbol{\Delta\phi}_0\mathbf{y}$. It is unbiased, but, in general, not the best.

The second consequence of the randomization of blocks is contained in the dispersion structure of $\mathbf{y}$. Now, it can be expressed (cf. Kala, 1991) as

$$D(\mathbf{y}) = \frac{1}{b}\sum_{j=1}^{b} \sigma^2_{u.j}\{\mathbf{I} - (1/k_j)\mathbf{D}'\mathbf{D}\} + \sigma^2_b\{\mathbf{D}'\mathbf{D} - (1/b)\mathbf{1}\mathbf{1}'\} + \sigma^2\mathbf{I}, \tag{15}$$

where σ_b^2 is a variance between blocks. The variance components $\sigma_{u.j}^2$, $j = 1, 2, ..., b$, reflecting the variability of plots inside blocks, are spread here over all units, rather than are located in diagonal subblocks, as it was in (10).

In the model with expectation (13) and dispersion matrix (15), the existence of BLUE does not depend on the relation between the unknown variance components $\sigma_{u.j}^2$, $j = 1, 2, ..., b$, but it depends on the design. In particular, if $R(\mathbf{D}'\mathbf{D}\boldsymbol{\phi}_0\boldsymbol{\Delta}') \subseteq R(\boldsymbol{\Delta}')$, the BLUE exists for all treatment contrasts $\mathbf{C}_0\boldsymbol{\tau}$, which coincides with its least squares estimator $\boldsymbol{\Delta}\boldsymbol{\phi}_0\mathbf{y}$. When we restrict to the contrasts $\mathbf{C}\boldsymbol{\tau}$, then $\boldsymbol{\Delta}\boldsymbol{\phi}\mathbf{y}$ will be their best estimator, if $R(\boldsymbol{\phi}\boldsymbol{\Delta}') \subseteq R(\boldsymbol{\Delta}')$. Thus, the most promising statistics can be the BLUEs in the model with complete randomization only under special conditions.

8. Intra block model

In almost all cases we have transformed the vector of observations $\mathbf{y}$ by the orthogonal projection $\boldsymbol{\phi}$ defined in (5). The expectation of the resulting vector has the form

$$E(\boldsymbol{\phi}\mathbf{y}) = \boldsymbol{\phi}\boldsymbol{\Delta}'\boldsymbol{\tau}, \tag{16}$$

which is the same for all considered models. The dispersion matrix of the transformed observations $\boldsymbol{\phi}\mathbf{y}$ depends on the assumed dispersion matrix $D(\mathbf{y})$. But it is proportional to the matrix $\boldsymbol{\phi}$ for the fixed model, the model with randomized plots and homogeneous variances $\sigma_{u.j}^2$, $j = 1, 2, ..., b$, and for the model with complete randomization. Let us say, it has the form

$$D(\boldsymbol{\phi}\mathbf{y}) = \alpha^2\boldsymbol{\phi}, \tag{17}$$

where α^2 is an unknown variance. This is the intra-block model (cf. Caliński and Kageyama, 1988, 1991). In such a model the BLUE of $\mathbf{C}\boldsymbol{\tau}$ exists. It coincides with the least squares estimator $\boldsymbol{\Delta}\boldsymbol{\phi}\mathbf{y}$, and has the dispersion matrix proportional to the matrix $\mathbf{C}$. Thus, the variance balance property preserves sense and the criterion of Theorem 6 can be applied.

9. Conclusions

Throughout the previous sections we have discussed six leading results from the block design theory. They were related to connectedness (Theorem 1), estimability (Theorems 2 and 3), best estimation (Theorems 4 and 5), and balance (Theorem 6). All of them involve the matrix $\mathbf{C}$ of the design. The designs, however, can be modeled differently, depending on the knowledge about the experimental material and the applied randomization procedure. The validity of the results in different models is marked in Table 1.

Table 1. Validity of Theorems 1 - 6 in different models

Model	$E(\mathbf{y})$	$D(\mathbf{y})$	Theorem 1	2	3	4	5	6
Standard	(6)	$\sigma^2\mathbf{I}$	√	√	√	√	√	√
Randomized plots	(6)	(10)	√	√	√	not[1)]	not	not
Randomized plots with (11)	(6)	(12)	√	√	√	√	√	√
Completely randomized	(13)	(15)	√	not[2)]	not[2)]	not[3)]	not	not
Intra-block	(16)	(17)	√	√	√	√	√	√

[1)] BLUE does not exist

[2)] All contrasts are estimable

[3)] BLUE exists in special designs only

Summing up the above discussion we can say that connectedness is not always equivalent to estimability of all treatment contrasts. The model with complete randomization is the exception. Moreover, we can observe that the classic least squares method confirms its usefulness. In the cases of three models, it gives the BLUE. In the case of the model with randomized plots, the BLUE, in general, does not exist, however, the least squares method supplies the reasonable unbiased estimates. In the model with complete randomization, the existence of the BLUE is limited by special conditions. But, if they are satisfied, the BLUE again follows from the least squares method. Such a conclusion can also be drawn from the fact that in all models, except the intra-block one, the set of admitted dispersion matrices involves $\sigma^2\mathbf{I}$. If the BLUE exists in such case, it must be equal to the least squares estimate (cf. Kala, 1981, 1990).

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Received 15 August 1998

O własnościach i modelach w teorii układów blokowych

STRESZCZENIE

Teoria układów blokowych obejmuje kilka ogólnych idei, wiele własności i szereg różnych modeli. W pracy ukazano łączące je związki, a w szczególności ujawniono ich sens i przydatność w nawiązaniu do konkretnych warunków eksperymentalnych. Rozważania rozpoczyna klasyczny model z efektami stałymi, który wydaje się stanowić podstawę całej teorii. Pracę kończą modele mieszane uwzględniające randomizację, które były szeroko dyskutowane w ostatnich dziesięciu latach przez Profesora Tadeusza Calińskiego.

SŁOWA KLUCZOWE: spójność, estymowalność, najlepszy nieobciążony estymator liniowy, zrównoważenie ze względu na wariancję, randomizacja.