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Recovery of inter-block information when the experiment is in a nested block design

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SUMMARY

A general randomization model for experiments in nested block designs is considered from the point of view of the recovery of inter-block information. First, it is shown how under the model the best linear unbiased estimators of treatment parametric functions can be obtained when the variance components are known. Then, a general method of estimating these, usually unknown, variance components is described and properties of the resulting empirical estimators of treatment parametric functions are examined. Some approximation of the variance of any such estimator is considered under certain design conditions. The paper extends to nested block designs the relevant results known for ordinary block designs (with one stratum of blocks).

KEY WORDS: best linear unbiased estimation, estimation of variance components, nested block designs, randomization model, recovery of inter-block information.

1. Introduction and preliminaries

In a recent paper by Caliński and Kageyama (1996a) the recovery of inter-block information in estimating parametric functions under a randomization model for experiments with one stratum of blocks of experimental units (plots) has been presented and discussed. The results there are, however, not directly applicable to experiments in which the available blocks are further grouped into some superblocks, i.e., form two strata of blocks, one nested in the other. Experimental designs with such nested blocks are used quite often in practice. Common examples are the lattice designs introduced by Yates (1936, 1939) or, more generally, the so-called resolvable block designs (see, e.g., Caliński and Kageyama, 1996b, Sections 4.2 and 4.3). The randomization model for experiments in so extended block designs, called "nested block (NB) designs", has been considered by Caliński (1994), but without tackling the problem of combining information from the various strata. The purpose of the present paper is, therefore, to reconsider that randomization model from the point of view of the recovery of inter-block information. In that way the present paper will supplement the earlier paper by Caliński (1994) and extend the results given recently by Caliński and Kageyama (1996a) to a general NB design.

The notation and terminology of the present paper is the same or similar to that used in the two earlier papers, mentioned above. Thus, a block design for v treatments in b blocks is described by its $v \times b$ incidence matrix $\mathbf{N} = \mathbf{\Delta D}'$, where $\mathbf{\Delta}'$ is the $n \times v$ design matrix for treatments and $\mathbf{D}'$ is the $n \times b$ design matrix for blocks. Such design is denoted by D^*. Suppose that the blocks of D^*, called also sub-blocks, are grouped into superblocks, say a in number. This can be reflected by the partitions $\mathbf{\Delta} = [\mathbf{\Delta}_1 : ... : \mathbf{\Delta}_a]$, $\mathbf{D} = \text{diag}\,[\mathbf{D}_1 : ... : \mathbf{D}_a]$, and, consequently, $\mathbf{N} = [\mathbf{N}_1 : ... : \mathbf{N}_a]$, where $\mathbf{\Delta}_h$, $\mathbf{D}_h$ and $\mathbf{N}_h = \mathbf{\Delta}_h \mathbf{D}_h'$ describe a component design, denoted by D_h, confined to superblock h $(h = 1, ..., a)$. The resulting design laying out the v treatments in the a superblocks is then denoted by D and described by its $v \times a$ incidence matrix $\mathbf{M} = \mathbf{\Delta G}'$, where $\mathbf{G}'$ is the $n \times a$ design matrix for superblocks, of the form

$$\mathbf{G}' = \mathbf{D}'\text{diag}[\mathbf{1}_{b_1} : ... : \mathbf{1}_{b_a}] = \text{diag}[\mathbf{1}_{n_1} : ... : \mathbf{1}_{n_a}], \tag{1.1}$$

with b_h denoting the number of blocks in superblock h, and n_h the number of units in that superblock, i.e., its size. Note that $n_h = \mathbf{1}_{b_h}' \mathbf{k}_h$, if $\mathbf{k}_h = [k_{1(h)}, ..., k_{b_h(h)}]'$ denotes the vector of block sizes in superblock h. One can also write $\mathbf{M} = [\mathbf{r}_1 : ... : \mathbf{r}_a]$, with $\mathbf{r}_h$ denoting the vector of treatment replications in superblock h. (Therefore the matrix $\mathbf{M}$ has been denoted by $\mathbf{R}$ in Caliński, 1994, p. 47). Evidently, $\mathbf{N1}_b = \mathbf{M1}_a = \mathbf{r}$ is the vector of treatment replications in the whole NB design, as well as in D^* and D, $\mathbf{N}'\mathbf{1}_v = \mathbf{k} = [\mathbf{k}_1', ..., \mathbf{k}_a']'$ is the vector of block sizes in D^*, $\mathbf{M}'\mathbf{1}_v = \mathbf{n} = [n_1, ..., n_a]'$ is the vector of superblock sizes in D. Similarly as $\mathbf{r}^\delta = \mathbf{\Delta\Delta}'$ and $\mathbf{k}^\delta = \mathbf{DD}'$ are the diagonal matrices of treatment replications and block sizes, respectively, $\mathbf{n}^\delta = \mathbf{GG}'$ is the diagonal matrix of superblock sizes. The total number of units used in the experiment is $n = \mathbf{1}_v'\mathbf{r} = \mathbf{1}_b'\mathbf{k} = \mathbf{1}_a'\mathbf{n}$.

Furthermore, distinction is made between the potential (or available) number of superblocks, N_A, from which a choice can be made, and the number a of those actually chosen for the experiment. The usual situation is that $a = N_A$, but in general $a \leq N_A$. Similarly, it is convenient to distinct between the potential (available) number of blocks within a superblock and the number of those of them actually chosen to the experiment. Finally, a distinction is made between the potential number of units (plots) within a block and the number of those of them actually used in the experiment.

2. The randomization model

While in an ordinary block design the stratification of the experimental units leads to three strata, of units within blocks, of blocks within the total experimental area, and of the total area (cf. Caliński and Kageyama, 1991, p. 105), in the extended situation to be considered here four strata can be distinguished. Those are of units within blocks, of blocks within superblocks, of superblocks within the total experimental area, and of the total area. Consequently, the extended randomization model has to take into account three instead of two stages of randomization, viz., of units within blocks, of blocks within superblocks and of the latter within the total area.

The randomization model for experiments in NB designs has been considered by Caliński (1994) and also by Mejza and Kageyama (1995). It differs from the randomization model for ordinary block design, considered by Caliński and Kageyama (1991, 1996a), by the addition of the component $\mathbf{G}'\boldsymbol{\alpha}$, where $\mathbf{G}'$ is the design matrix for superblocks, defined in (1.1), and $\boldsymbol{\alpha}$ is an $a \times 1$ vector of superblock random effects. Thus, with this component, the model can be written in matrix notation as

$$\mathbf{y} = \boldsymbol{\Delta}'\boldsymbol{\tau} + \mathbf{G}'\boldsymbol{\alpha} + \mathbf{D}'\boldsymbol{\beta} + \boldsymbol{\eta} + \mathbf{e}, \tag{2.1}$$

where $\mathbf{y} = [\mathbf{y}'_1, ..., \mathbf{y}'_a]'$ is an $n \times 1$ vector of observed variables, with $\mathbf{y}_h$ representing the variables observed on n_h units of the superblock h, $\boldsymbol{\tau}$ is a $v \times 1$ vector of treatment parameters, $\boldsymbol{\beta} = [\boldsymbol{\beta}'_1, ..., \boldsymbol{\beta}'_a]'$ is a $b \times 1$ vector of block random effects, with $\boldsymbol{\beta}_h$ representing the effects of the b_h blocks in the superblock h, and where $\boldsymbol{\eta}$ and $\mathbf{e}$ are the corresponding $n \times 1$ vectors of unit error and technical error random variables, respectively. The expectation vector remains unchanged, i.e.,

$$\mathrm{E}(\mathbf{y}) = \boldsymbol{\Delta}'\boldsymbol{\tau}, \tag{2.2}$$

while the dispersion matrix is of the extended form

$$\begin{aligned}\mathrm{Cov}(\mathbf{y}) \ &= \ (\mathbf{G}'\mathbf{G} - N_A^{-1}\mathbf{1}_n\mathbf{1}'_n)\sigma_A^2 + (\mathbf{D}'\mathbf{D} - B_H^{-1}\mathbf{G}'\mathbf{G})\sigma_B^2 \\ &\quad + (\mathbf{I}_n - K_H^{-1}\mathbf{D}'\mathbf{D})\sigma_U^2 + \mathbf{I}_n\sigma_e^2,\end{aligned} \tag{2.3}$$

where N_A is the number of available superblocks, and B_H is a weighted harmonic average of the available numbers of blocks $(B_1, ..., B_{N_A})$ within the N_A available superblocks, similarly as K_H is such an average of the available numbers of units within the $B_1 + ... + B_{N_A}$ available blocks, and where σ_A^2, σ_B^2, σ_U^2 and σ_e^2 are the variance components related to the random vectors $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\eta}$ and $\mathbf{e}$, respectively, all these quantities being defined precisely in Caliński (1994, Section 2.1). Since (2.3) can also be written as

$$\mathrm{Cov}(\mathbf{y}) = \sigma_1^2(\mathbf{G}'\boldsymbol{\Gamma}_1\mathbf{G} + \mathbf{D}'\boldsymbol{\Gamma}_2\mathbf{D} + \mathbf{I}_n), \tag{2.4}$$

where

$$\mathbf{\Gamma}_1 = \mathbf{I}_a\gamma_1 - N_A^{-1}\mathbf{1}_a\mathbf{1}_a'\sigma_A^2/\sigma_1^2,\ \gamma_1 = (\sigma_A^2 - B_H^{-1}\sigma_B^2)/\sigma_1^2,\ \sigma_1^2 = \sigma_U^2 + \sigma_e^2 \qquad (2.5)$$

and

$$\mathbf{\Gamma}_2 = \mathbf{I}_b\gamma_2, \quad \gamma_2 = (\sigma_B^2 - K_H^{-1}\sigma_U^2)/\sigma_1^2, \qquad (2.6)$$

the combined analysis of an experiment in an NB design can be seen as a straightforward, though not very simple, extension of that described for an ordinary block design (i.e., with one stratum of blocks) by Caliński and Kageyama (1996a, Section 3). Details of this extension will be presented in the next section.

3. Recovery of inter-block information in a general NB design

The main estimation results obtained for NB designs by Caliński (1994, Section 2.2) show that unless the estimated function $\mathbf{c}'\boldsymbol{\tau}$ satisfies certain quite restrictive conditions, there does not exist the best linear unbiased estimator (BLUE) of it under the randomization model (2.1). However (cf. Caliński, 1994, Section 3), in many, though not in all, cases the estimation of a contrast of treatment parameters, $\mathbf{c}'\boldsymbol{\tau}$, can be based on information available in two or three of the experimental strata. Unfortunately, each of them provides a separate estimate of the contrast, often of quite different value. Therefore, a natural question arising in this context is whether and how it is possible to utilize the information from various strata to obtain a single estimate in a somehow optimal way. Caliński and Kageyama (1996a) have considered this for a general, but ordinary, block design, where the combination of information concerns two strata only. Here an extension of their results will be presented in a way applicable to any NB design for which the general randomization model (2.1) is appropriate.

3.1. The BLUEs under known variance components

First let the problem be considered under an unrealistic assumption that the variance components appearing in the dispersion matrix (2.3) are known, or at least their ratios γ_1 and γ_2 defined in (2.5) and (2.6) are known. Then the following results are essential (cf. Caliński and Kageyama, 1996a, Section 3.1).

LEMMA 3.1. *Let the model be as in* (2.1), *with the expectation vector* (2.2) *and the dispersion matrix* (2.3), *the latter written equivalently as in* (2.4). *Furthermore, suppose that the true values of* γ_1 *and* γ_2 *are known. Then,*

(a) *any function* $\mathbf{w}'\mathbf{y}$ *which is the BLUE of its expectation,*

(b) *a vector which is the BLUE of* $\mathrm{E}(\mathbf{y}) = \mathbf{\Delta}'\boldsymbol{\tau}$ *and, hence,*

(c) *a vector which gives the residuals,*

all remain unchanged when altering the present model by deleting $N_A^{-1}(\sigma_A^2/\sigma_1^2)\mathbf{1}_a\mathbf{1}_a'$

in (2.5), *i.e., by reducing* (2.4) *to*

$$\mathrm{Cov}(\mathbf{y}) = \sigma_1^2(\gamma_1\mathbf{G}'\mathbf{G} + \gamma_2\mathbf{D}'\mathbf{D} + \mathbf{I}_n) = \sigma_1^2\mathbf{T}, \tag{3.1}$$

where $\mathbf{T} = \gamma_1\mathbf{G}'\mathbf{G} + \gamma_2\mathbf{D}'\mathbf{D} + \mathbf{I}_n$. *The matrix* $\mathbf{T}$ *is positive definite (p.d.) if* $\gamma_1 \geq 0$ *and* $\gamma_2 > -1/k_{\max}$, *where* $k_{\max} = \max_{j(h)} k_{j(h)}$.

Proof. Note that, with $\mathbf{P}_{\mathbf{\Delta}'} = \mathbf{\Delta}'\mathbf{r}^{-\delta}\mathbf{\Delta}$, the equality $(\mathbf{G}'\mathbf{\Gamma}_1\mathbf{G} + \mathbf{D}'\mathbf{\Gamma}_2\mathbf{D} + \mathbf{I}_n)(\mathbf{I}_n - \mathbf{P}_{\mathbf{\Delta}'}) = (\gamma_1\mathbf{G}'\mathbf{G} + \gamma_2\mathbf{D}'\mathbf{D} + \mathbf{I}_n)(\mathbf{I}_n - \mathbf{P}_{\mathbf{\Delta}'})$ holds. This implies that (a) the relevant condition for $\mathbf{w}$, given in Theorem 3 of Zyskind (1967), is satisfied under the original model if and only if it is satisfied under the alternative model with (3.1), and that (b) the BLUE of $\mathbf{\Delta}'\boldsymbol{\tau}$, as given by Rao (1974, Theorem 3.2), remains unchanged when (2.4) is replaced by (3.1), so that also (c) the residual vector is unchanged then. The matrix $\mathbf{T}$ in (3.1) is p.d. if $\gamma_1 \geq 0$ and $\gamma_2 > -\mathbf{x}'\mathbf{x}/\mathbf{x}'\mathbf{D}'\mathbf{D}\mathbf{x}$, for any vector $\mathbf{x}$, and the latter holds if $\gamma_2 > -1/\varkappa_{\max}$, where $\varkappa_{\max}$ is the maximum eigenvalue of $\mathbf{D}'\mathbf{D}$ (and of $\mathbf{D}\mathbf{D}'$), this being $k_{\max}$. (These assumptions on γ_1 and γ_2 are reasonable, as $\gamma_1 \geq 0$ if and only if $\sigma_A^2 \geq B_H^{-1}\sigma_B^2$, and for $\gamma_2 > -1/k_{\max}$ it is sufficient that $K_H \geq k_{\max}$ and $K_H\sigma_B^2 + \sigma_e^2 > 0$; of course $\gamma_2 \geq 0$ if and only if $\sigma_B^2 \geq K_H^{-1}\sigma_U^2$.) □

THEOREM 3.1. *Under the model and assumptions as in Lemma* 3.1, *including the assumption that* $\gamma_1 \geq 0$ *and* $\gamma_2 > -1/k_{\max}$,

(a) *the BLUE of* $\boldsymbol{\tau}$ *is of the form*

$$\hat{\boldsymbol{\tau}} = (\mathbf{\Delta}\mathbf{T}^{-1}\mathbf{\Delta}')^{-1}\mathbf{\Delta}\mathbf{T}^{-1}\mathbf{y}, \tag{3.2}$$

where $\mathbf{T}^{-1}$ *can be taken as*

$$\mathbf{T}^{-1} = \boldsymbol{\phi} + \mathbf{D}'\mathbf{k}^{-\delta}(\mathbf{k}^{-\delta} + \gamma_2\mathbf{I}_b + \gamma_1\mathrm{diag}[\mathbf{1}_{b_1}\mathbf{1}_{b_1}' : \ldots : \mathbf{1}_{b_a}\mathbf{1}_{b_a}'])^{-1}\mathbf{k}^{-\delta}\mathbf{D}, \tag{3.3}$$

with $\boldsymbol{\phi} = \mathbf{I}_n - \mathbf{D}'\mathbf{k}^{-\delta}\mathbf{D}$;

(b) *the dispersion matrix of* $\hat{\boldsymbol{\tau}}$ *is*

$$\mathrm{Cov}(\hat{\boldsymbol{\tau}}) = \sigma_1^2(\mathbf{\Delta}\mathbf{T}^{-1}\mathbf{\Delta}')^{-1} - N_A^{-1}\sigma_A^2\mathbf{1}_v\mathbf{1}_v'; \tag{3.4}$$

(c) *the BLUE of* $\mathbf{c}'\boldsymbol{\tau}$ *for any* $\mathbf{c}$ *is* $\mathbf{c}'\hat{\boldsymbol{\tau}}$, *with the variance* $\mathbf{c}'\mathrm{Cov}(\hat{\boldsymbol{\tau}})\mathbf{c}$, *which reduces to*

$$\mathrm{Var}(\widehat{\mathbf{c}'\boldsymbol{\tau}}) = \sigma_1^2\mathbf{c}'(\mathbf{\Delta}\mathbf{T}^{-1}\mathbf{\Delta}')^{-1}\mathbf{c}, \tag{3.5}$$

if $\mathbf{c}'\boldsymbol{\tau}$ *is a contrast;*

(d) *the minimum norm quadratic unbiased estimator (MINQUE) of* σ_1^2 *is*

$$\hat{\sigma}_1^2 = (n-v)^{-1}\,\|\mathbf{y} - \mathbf{\Delta}'\hat{\boldsymbol{\tau}}\|_{\mathbf{T}^{-1}}^2 = (n-v)^{-1}(\mathbf{y} - \mathbf{\Delta}'\hat{\boldsymbol{\tau}})'\mathbf{T}^{-1}(\mathbf{y} - \mathbf{\Delta}'\hat{\boldsymbol{\tau}}). \tag{3.6}$$

Proof. From Theorem 3.2(c) of Rao (1974), and Lemma 3.1 above, the BLUE of $\mathbf{\Delta}'\tau$ is $\widehat{\mathbf{\Delta}'\tau} = \mathbf{P}_{\mathbf{\Delta}';\mathbf{T}^{-1}}\mathbf{y}$, where $\mathbf{P}_{\mathbf{\Delta}';\mathbf{T}^{-1}} = \mathbf{\Delta}'(\mathbf{\Delta}\mathbf{T}^{-1}\mathbf{\Delta}')^{-1}\mathbf{\Delta}\mathbf{T}^{-1}$. Hence the result (3.2). This then implies (3.4), since (2.4) can be written as $\mathrm{Cov}(\mathbf{y}) = \sigma_1^2\mathbf{T} \dot{-} N_A^{-1}\sigma_A^2\mathbf{1}_n\mathbf{1}_n'$. Formula (3.5) follows from (3.4) directly, and formula (3.3) can easily be checked. Formula(3.6) follows from Theorem 3.4(c) of Rao (1974) by noting that the residual sum of squares is of the form

$$\|(\mathbf{I}_n - \mathbf{P}_{\mathbf{\Delta}';\mathbf{T}^{-1}})\mathbf{y}\|^2_{\mathbf{T}^{-1}} = \mathbf{y}'(\mathbf{I}_n - \mathbf{P}_{\mathbf{\Delta}';\mathbf{T}^{-1}})'\mathbf{T}^{-1}(\mathbf{I}_n - \mathbf{P}_{\mathbf{\Delta}';\mathbf{T}^{-1}})\mathbf{y}, \tag{3.7}$$

equivalent to (3.13) of Rao (1974), which provides the MINQUE of $d\sigma_1^2$, where $d = \mathrm{rank}(\mathbf{T} : \mathbf{\Delta}') - \mathrm{rank}(\mathbf{\Delta}') = n - v$. □

Note that ϕ in (3.3) is responsible for the intra-block information, while the term following it takes care of the inter-block information, with γ_2 responsible for that within the superblocks and with γ_1 for that between the superblocks, the maximum recovery of the former information being achieved at $\gamma_2 \leq 0$ and that of the latter at $\gamma_1 = 0$.

3.2. The estimation of unknown variance ratios

Results established in Section 3.1 are based on the assumption that the ratios γ_1 and γ_2 are known (see Lemma 3.1). In practice, however, this is usually not the case. Therefore, to make the theory applicable, estimators not only of σ_1^2 but also of γ_1 and γ_2 are needed. Although there may be various approaches adopted for finding these estimators, that utilized in Caliński and Kageyama (1996a) seems to be particularly suitable. Let its extension for NB designs be presented here in details.

First let the residual sum of squares (3.7) be written as

$$\begin{aligned} \|(\mathbf{I}_n - \mathbf{P}_{\mathbf{\Delta}';\mathbf{T}^{-1}})\mathbf{y}\|^2_{\mathbf{T}^{-1}} &= \mathbf{y}'\mathbf{RTRy} \\ &= \gamma_1\mathbf{y}'\mathbf{RG}'\mathbf{GRy} + \gamma_2\mathbf{y}'\mathbf{RD}'\mathbf{DRy} + \mathbf{y}'\mathbf{RRy}, \end{aligned} \tag{3.8}$$

where

$$\mathbf{R} = \mathbf{T}^{-1}(\mathbf{I}_n - \mathbf{P}_{\mathbf{\Delta}';\mathbf{T}^{-1}}) = \mathbf{T}^{-1} - \mathbf{T}^{-1}\mathbf{\Delta}'(\mathbf{\Delta}\mathbf{T}^{-1}\mathbf{\Delta}')^{-1}\mathbf{\Delta}\mathbf{T}^{-1}. \tag{3.9}$$

Equating then the partial sums of squares in (3.8) to their expectations, one obtains the set of equations

$$\begin{bmatrix} \mathrm{tr}(\mathbf{RG}'\mathbf{GRG}'\mathbf{G}) & \mathrm{tr}(\mathbf{RG}'\mathbf{GRD}'\mathbf{D}) & \mathrm{tr}(\mathbf{RG}'\mathbf{GR}) \\ \mathrm{tr}(\mathbf{RD}'\mathbf{DRG}'\mathbf{G}) & \mathrm{tr}(\mathbf{RD}'\mathbf{DRD}'\mathbf{D}) & \mathrm{tr}(\mathbf{RD}'\mathbf{DR}) \\ \mathrm{tr}(\mathbf{RG}'\mathbf{GR}) & \mathrm{tr}(\mathbf{RD}'\mathbf{DR}) & \mathrm{tr}(\mathbf{RR}) \end{bmatrix} \begin{bmatrix} \sigma_1^2\gamma_1 \\ \sigma_1^2\gamma_2 \\ \sigma_1^2 \end{bmatrix} = $$

$$= \begin{bmatrix} \mathbf{y}'\mathbf{RG}'\mathbf{GRy} \\ \mathbf{y}'\mathbf{RD}'\mathbf{DRy} \\ \mathbf{y}'\mathbf{RRy} \end{bmatrix} \tag{3.10}$$

from which estimators of $\sigma_1^2\gamma_1$, $\sigma_1^2\gamma_2$ and σ_1^2, and hence of γ_1 and γ_2, can be obtained. Exactly the same equations, as those in (3.10), follow from the MINQUE approach of Rao (1971). Also note that, on account of the equalities

$$\mathrm{tr}(\mathbf{RG'GRT}) = \mathrm{tr}(\mathbf{RG'G}), \quad \mathrm{tr}(\mathbf{RD'DRT}) = \mathrm{tr}(\mathbf{RD'D}) \quad \text{and} \quad \mathrm{tr}(\mathbf{RRT}) = \mathrm{tr}(\mathbf{R}),$$

the equations (3.10) can equivalently be written as

$$\mathbf{y'RG'GRy} = \sigma_1^2\mathrm{tr}(\mathbf{RG'G}),\ \mathbf{y'RD'DRy} = \sigma_1^2\mathrm{tr}(\mathbf{RD'D}),\ \mathbf{y'RRy} = \sigma_1^2\mathrm{tr}(\mathbf{R}), \quad (3.11)$$

and the equations (3.11) can be shown to coincide with those on which the so-called modified (or marginal) maximum likelihood (MML) estimation method is based, the method being also known as the restricted maximum likelihood (REML) approach (cf. Patterson and Thompson, 1975; Harville, 1977).

Clearly, the equations (3.10) have no direct analytic solution, since the matrix **R** itself contains the unknown parameters γ_1 and γ_2, as can be seen from (3.3) and (3.9). Therefore, to solve these equations, or any equivalence of them, an iterative procedure is to be applied (cf. Patterson and Thompson, 1971, Section 6). It starts with some preliminary estimates $\gamma_{1,0}$ and $\gamma_{2,0}$ incorporated into the equations (3.10) by changing the matrix **R** there to

$$\mathbf{R}_0 = \mathbf{T}_0^{-1} - \mathbf{T}_0^{-1}\mathbf{\Delta}'(\mathbf{\Delta}\mathbf{T}_0^{-1}\mathbf{\Delta}')^{-1}\mathbf{\Delta}\mathbf{T}_0^{-1}, \quad (3.12)$$

where

$$\mathbf{T}_0^{-1} = \boldsymbol{\phi} + \mathbf{D'k}^{-\delta}(\mathbf{k}^{-\delta} + \gamma_{2,0}\mathbf{I}_b + \gamma_{1,0}\mathrm{diag}[\mathbf{1}_{b_1}\mathbf{1}'_{b_1} : \ldots : \mathbf{1}_{b_a}\mathbf{1}'_{b_a}])^{-1}\mathbf{k}^{-\delta}\mathbf{D} \quad (3.13)$$

(with $\mathbf{T}_0^{-1} \to \boldsymbol{\phi}$ if $\gamma_{2,0} \to \infty$). However, instead of the equations so obtained, it is more convenient to solve iteratively their equivalence of the form

$$\begin{bmatrix} \mathrm{tr}(\mathbf{R}_0\mathbf{G'G}\mathbf{R}_0\mathbf{G'G}) & \mathrm{tr}(\mathbf{R}_0\mathbf{G'G}\mathbf{R}_0\mathbf{D'D}) & \mathrm{tr}(\mathbf{R}_0\mathbf{G'G}) \\ \mathrm{tr}(\mathbf{R}_0\mathbf{D'D}\mathbf{R}_0\mathbf{G'G}) & \mathrm{tr}(\mathbf{R}_0\mathbf{D'D}\mathbf{R}_0\mathbf{D'D}) & \mathrm{tr}(\mathbf{R}_0\mathbf{D'D}) \\ \mathrm{tr}(\mathbf{R}_0\mathbf{G'G}) & \mathrm{tr}(\mathbf{R}_0\mathbf{D'D}) & n-v \end{bmatrix} \begin{bmatrix} \sigma_1^2(\gamma_1 - \gamma_{1,0}) \\ \sigma_1^2(\gamma_2 - \gamma_{2,0}) \\ \sigma_1^2 \end{bmatrix} =$$

$$= \begin{bmatrix} \mathbf{y'R}_0\mathbf{G'GR}_0\mathbf{y} \\ \mathbf{y'R}_0\mathbf{D'DR}_0\mathbf{y} \\ \mathbf{y'R}_0\mathbf{y} \end{bmatrix}. \quad (3.14)$$

By solving the equations (3.14) one obtains the revised estimates of γ_1 and γ_2, which can be written as

$$\hat{\gamma}_1 = \gamma_{1,0} + \frac{a^{00}\mathbf{y'R}_0\mathbf{G'GR}_0\mathbf{y} + a^{01}\mathbf{y'R}_0\mathbf{D'DR}_0\mathbf{y} + a^{02}\mathbf{y'R}_0\mathbf{y}}{a^{20}\mathbf{y'R}_0\mathbf{G'GR}_0\mathbf{y} + a^{21}\mathbf{y'R}_0\mathbf{D'DR}_0\mathbf{y} + a^{22}\mathbf{y'R}_0\mathbf{y}} \quad (3.15)$$

and

$$\hat{\gamma}_2 = \gamma_{2,0} + \frac{a^{10}\mathbf{y}'\mathbf{R}_0\mathbf{G}'\mathbf{G}\mathbf{R}_0\mathbf{y}+a^{11}\mathbf{y}'\mathbf{R}_0\mathbf{D}'\mathbf{D}\mathbf{R}_0\mathbf{y}+a^{12}\mathbf{y}'\mathbf{R}_0\mathbf{y}}{a^{20}\mathbf{y}'\mathbf{R}_0\mathbf{G}'\mathbf{G}\mathbf{R}_0\mathbf{y}+a^{21}\mathbf{y}'\mathbf{R}_0\mathbf{D}'\mathbf{D}\mathbf{R}_0\mathbf{y}+a^{22}\mathbf{y}'\mathbf{R}_0\mathbf{y}}, \tag{3.16}$$

where

$$a^{00} = a_{11}a_{22} - a_{12}^2, \qquad a^{01} = a^{10} = a_{12}a_{02} - a_{01}a_{22},$$

$$a^{02} = a^{20} = a_{01}a_{12} - a_{11}a_{02}, \qquad a^{11} = a_{00}a_{22} - a_{02}^2,$$

$$a^{12} = a^{21} = a_{01}a_{02} - a_{00}a_{12}, \qquad a^{22} = a_{00}a_{11} - a_{01}^2,$$

with

$$a_{00} = \mathrm{tr}[(\mathbf{G}\mathbf{R}_0\mathbf{G}')^2], \quad a_{01} = \mathrm{tr}(\mathbf{D}\mathbf{R}_0\mathbf{G}'\mathbf{G}\mathbf{R}_0\mathbf{D}'), \quad a_{02} = \mathrm{tr}(\mathbf{G}\mathbf{R}_0\mathbf{G}'),$$

$$a_{11} = \mathrm{tr}[(\mathbf{D}\mathbf{R}_0\mathbf{D}')^2], \quad a_{12} = \mathrm{tr}(\mathbf{D}\mathbf{R}_0\mathbf{D}') \quad \text{and} \quad a_{22} = n - v.$$

Thus, a single iteration of the iterative method (which extends that of Patterson and Thompson, 1971, p.550) consists here of the following two steps:

(0) One starts with some preliminary estimates $\gamma_{1,0}$ (≥ 0) and $\gamma_{2,0}$ ($> -1/k_{\max}$) of γ_1 and γ_2, respectively, to obtain the equations (3.14).

(1) By solving (3.14), revised estimates of γ_1 and γ_2 are obtained in the form (3.15) and (3.16), respectively, and these are then used as new preliminary estimates in step (0) of the next iteration.

However, it should always be observed that the original as well as the new preliminary estimates satisfy the conditions $\gamma_{1,0} \geq 0$ and $\gamma_{2,0} > -1/k_{\max}$. Therefore, if any of the formulae (3.15) and (3.16) gives a revised estimate not satisfying these bounds, the result is to be adjusted before entering step (0), in a way similar to that given in Caliński and Kageyama (1996a, p.367), following the suggestion of Rao and Kleffe (1988, p.237).

The described iteration is to be repeated until convergence, i.e., until the equalities

$$\frac{\mathbf{y}'\mathbf{R}_0\mathbf{G}'\mathbf{G}\mathbf{R}_0\mathbf{y}}{\mathrm{tr}(\mathbf{G}\mathbf{R}_0\mathbf{G}')} = \frac{\mathbf{y}'\mathbf{R}_0\mathbf{D}'\mathbf{D}\mathbf{R}_0\mathbf{y}}{\mathrm{tr}(\mathbf{D}\mathbf{R}_0\mathbf{D}')} = \frac{\mathbf{y}'\mathbf{R}_0\mathbf{y}}{n-v}$$

are reached. The values $\hat{\gamma}_1 = \gamma_{1,0}$ and $\hat{\gamma}_2 = \gamma_{2,0}$ satisfying them are then considered as the final estimates of γ_1 and γ_2, respectively, and the resulting ratio $\hat{\sigma}_1^2 = \mathbf{y}'\hat{\mathbf{R}}\mathbf{y}/(n-v)$, with $\hat{\mathbf{R}} = \mathbf{R}_0$ obtained according to (3.12) but after replacing $\gamma_{1,0}$ and $\gamma_{2,0}$ in (3.13) by the final values $\hat{\gamma}_1$ and $\hat{\gamma}_2$, respectively, can be considered as the final estimate of σ_1^2. Although the convergence of this process has not been proved, some experiences (cf., e.g., Rao and Kleffe, 1988, p.226) indicate that the procedure should work well in practice.

Now, inserting in formula (3.2), instead of $\mathbf{T}^{-1}$, the matrix $\hat{\mathbf{T}}^{-1}$ resulting from the replacements in (3.13) made as described above, an empirical estimator

$$\widetilde{\boldsymbol{\tau}} = (\boldsymbol{\Delta}\hat{\mathbf{T}}^{-1}\boldsymbol{\Delta}')^{-1}\boldsymbol{\Delta}\hat{\mathbf{T}}^{-1}\mathbf{y} \tag{3.17}$$

is obtained. The adjective "empirical" is used here to indicate that the unknown variance ratios γ_1 and γ_2 appearing in $\mathbf{T}$ have been replaced by their empirical estimates (cf. Rao and Kleffe, 1988, Section 10.5). Of course, (3.17) is not the same as the BLUE (3.2) obtainable with the exact values of γ_1 and γ_2.

3.3. Properties of the empirical estimators

To gain an insight into the properties of the empirical estimator (3.17) of $\boldsymbol{\tau}$ and, hence, of such estimator of any parametric function $\mathbf{c}'\boldsymbol{\tau}$, use can be made of the approximation suggested by Kackar and Harville (1984). Its application becomes straightforward when it is possible to represent $\widetilde{\boldsymbol{\tau}}$ in terms of some simple linear functions of the observed vector $\mathbf{y}$, as shown by Caliński and Kageyama (1996) for experiments with one stratum of blocks. For NB designs such representation is not readily available in the general case. However, it can easily be obtained if the design satisfies the following two conditions:

(i) the design with respect to sub-blocks, D^*, described by $\mathbf{N}$, is proper (equiblock-sized), i.e., $\mathbf{k} = k\mathbf{1}_b$, and

(ii) the design with respect to superblocks, D, described by $\mathbf{M}$, is connected, proper and orthogonal, i.e., $\mathbf{M} = a^{-1}\mathbf{r}\mathbf{1}'_a$.

The above conditions imply, among others, that $n_1 = ... = n_a = n_0$ $(= n/a)$ and that $b_1 = ... = b_a = b_0$ $(= b/a = n_0/k)$.

In fact, the possibility of obtaining a simple representation of the estimator (3.17) in terms of linear functions of $\mathbf{y}$ depends on the availability of a suitable spectral decomposition of the matrix $\boldsymbol{\phi}_*\mathbf{T}\boldsymbol{\phi}_*$, where $\boldsymbol{\phi}_* = \mathbf{I}_n - \boldsymbol{\Delta}'\mathbf{r}^{-\delta}\boldsymbol{\Delta}$ and where $\mathbf{T}$ is as in (3.1). For this it is required that the component matrices in

$$\boldsymbol{\phi}_*\mathbf{T}\boldsymbol{\phi}_* = \gamma_1\boldsymbol{\phi}_*\mathbf{G}'\mathbf{G}\boldsymbol{\phi}_* + \gamma_2\boldsymbol{\phi}_*\mathbf{D}'\mathbf{D}\boldsymbol{\phi}_* + \boldsymbol{\phi}_* \tag{3.18}$$

commute in pairs. Each of the first two on the right-hand side in (3.18) commutes with $\boldsymbol{\phi}_*$ always. If the conditions (i) and (ii) hold, then also the first two commute one with the other. Although these conditions may seem restrictive, it can be claimed that a large number of NB designs used in practice satisfies (i) and (ii). For those which do not, the method described here needs further elaboration, but this will not be considered in the present paper.

Thus, from now on it is assumed that the NB design under consideration satisfies the above conditions (i) and (ii). This allows to obtain not only the decomposition

$$\phi_* \mathbf{D}'\mathbf{D}\phi_* = \sum_{j=1}^{h_*} \lambda_j \mathbf{v}_j \mathbf{v}_j' \tag{3.19}$$

[cf. (3.25) in Caliński and Kageyama (1996a)], but also

$$\phi_* \mathbf{G}'\mathbf{G}\phi_* = \sum_{j=1}^{g_*} \varkappa_j \mathbf{v}_j \mathbf{v}_j', \tag{3.20}$$

where, simultaneously, the vectors $\mathbf{v}_j$, $j = 1, ..., g_*, ..., h_*, ..., n - v$, are orthonormal eigenvectors of the matrix ϕ_*, corresponding to the unit eigenvalues of it, and where $g_* = \operatorname{rank}(\mathbf{G}\phi_*\mathbf{G}')$ and $h_* = \operatorname{rank}(\mathbf{D}\phi_*\mathbf{D}')$. Note that $\mathbf{G}\phi_*\mathbf{G}' = \mathbf{n}^\delta - \mathbf{M}'\mathbf{r}^{-\delta}\mathbf{M}$ is a dual of the matrix $\mathbf{r}^\delta - \mathbf{M}\mathbf{n}^{-\delta}\mathbf{M}'$ of rank g (say) and $\mathbf{D}\phi_*\mathbf{D}' = \mathbf{k}^\delta - \mathbf{N}'\mathbf{r}^{-\delta}\mathbf{N}$ is a dual of the matrix $\mathbf{r}^\delta - \mathbf{N}\mathbf{k}^{-\delta}\mathbf{N}'$ of rank h_1 (say; cf. Caliński, 1994, p. 58). Hence, in general, $g_* = a - v + g$ and $h_* = b - v + h_1$. Here, under (i) and (ii), $g = v - 1$ and, hence, $g_* = a - 1$. If, in addition, the design D^* is connected, then $h_1 = v - 1$ and $h_* = b - 1$. It can also be shown that, under (i) and (ii),

$$\lambda_1 = ... = \lambda_{g_*} = k \qquad \text{and} \qquad \varkappa_1 = ... = \varkappa_{g_*} = n_0 (= b_0 k).$$

Now, with (3.19) and (3.20) obtained under the conditions (i) and (ii), the spectral decomposition of $\phi_*\mathbf{T}\phi_*$ gets the form

$$\begin{aligned} \phi_*\mathbf{T}\phi_* &= (\gamma_1 n_0 + \gamma_2 k + 1) \sum_{j=1}^{g_*} \mathbf{v}_j\mathbf{v}_j' \\ &+ \sum_{j=g_*+1}^{h_*} (\gamma_2\lambda_j + 1)\mathbf{v}_j\mathbf{v}_j' + \sum_{j=h_*+1}^{n-v} \mathbf{v}_j\mathbf{v}_j', \end{aligned} \tag{3.21}$$

and, since the Moore-Penrose inverse of $\phi_*\mathbf{T}\phi_*$ can be shown to be equal to $\mathbf{R}$ [see (3.9)], it follows from (3.21) that

$$\begin{aligned} \mathbf{R} &= (\phi_*\mathbf{T}\phi_*)^+ = (\gamma_1 n_0 + \gamma_2 k + 1)^{-1} \sum_{j=1}^{g_*} \mathbf{v}_j\mathbf{v}_j' \\ &+ \sum_{j=g_*+1}^{h_*} (\gamma_2\lambda_j + 1)^{-1}\mathbf{v}_j\mathbf{v}_j' + \sum_{j=h_*+1}^{n-v} \mathbf{v}_j\mathbf{v}_j'. \end{aligned} \tag{3.22}$$

From (3.9) and (3.22) the estimator (3.17) can now be written as

$$\begin{aligned}\widetilde{\boldsymbol{\tau}} &= \hat{\boldsymbol{\tau}} + \mathbf{r}^{-\delta}\boldsymbol{\Delta}(\mathbf{TR} - \hat{\mathbf{T}}\hat{\mathbf{R}})\mathbf{y} = \hat{\boldsymbol{\tau}} + \mathbf{r}^{-\delta}\mathbf{ND}\left[\xi^{-1}\sum_{j=1}^{g_*}\mathbf{v}_j z_j + \sum_{j=g_*+1}^{h_*}\zeta_j^{-1}\mathbf{v}_j z_j\right] \\ &= \hat{\boldsymbol{\tau}} + \mathbf{r}^{-\delta}\mathbf{ND}\sum_{j=g_*+1}^{h_*}\zeta_j^{-1}\mathbf{v}_j z_j,\end{aligned}$$

since, under (i) and (ii), $\mathbf{NDv}_j = \mathbf{0}$ for $j = 1, ..., g_*$, where

$$\xi = \gamma_1 n_0 + \gamma_2 k + 1, \qquad \zeta_j = \gamma_2\lambda_j + 1,$$

and where

$$z_j = \frac{\gamma_1 b_0 + \gamma_2 - (\hat{\gamma}_1 b_0 + \hat{\gamma}_2)}{\hat{\gamma}_1 n_0 + \hat{\gamma}_2 k + 1}\mathbf{v}_j'\mathbf{y} \qquad \text{for} \qquad j = 1, ..., g_* \tag{3.23}$$

and

$$z_j = \frac{\gamma_2 - \hat{\gamma}_2}{\hat{\gamma}_2\lambda_j + 1}\mathbf{v}_j'\mathbf{y} \qquad \text{for} \qquad j = g_* + 1, ..., h_*. \tag{3.24}$$

The relevant representation of $\widetilde{\mathbf{c}'\boldsymbol{\tau}} = \mathbf{c}'\widetilde{\boldsymbol{\tau}}$ is then obvious.

Now, Lemma 3.2 of Caliński and Kageyama (1996a) can be extended as follows.

LEMMA 3.2. *Let the model of the variables observed in an NB design satisfying the conditions* (i) *and* (ii) *be as in* (2.1) *and suppose that the values of* γ_1 *and* γ_2 *in* (2.4) *are unknown, except that they satisfy the limits given in Theorem* 3.1 (*to secure that* $\mathbf{T}$ *is p.d.*), *the same being satisfied by their estimates* (*to secure that* $\hat{\mathbf{T}}$ *is p.d.*). *Furthermore, let the random variables* $\{z_j\}$ *defined in* (3.23) *and* (3.24) *satisfy the conditions*

$$\mathrm{E}(z_j) = 0, \qquad \mathrm{E}(z_j z_{j'}) = 0 \quad \text{and} \quad \mathrm{Var}(z_j) < \infty$$

for all j *and* $j' \neq j$ $(= 1, ..., h_*)$ *and for all admissible values of* γ_1 *and* γ_2. *Then the estimator* $\widetilde{\boldsymbol{\tau}}$ *has the properties*

$$\mathrm{E}(\widetilde{\boldsymbol{\tau}}) = \mathrm{E}(\hat{\boldsymbol{\tau}}) = \boldsymbol{\tau} \tag{3.25}$$

and

$$\mathrm{Cov}(\widetilde{\boldsymbol{\tau}}) = \mathrm{Cov}(\hat{\boldsymbol{\tau}}) + \mathbf{r}^{-\delta}\mathbf{ND}\sum_{j=g_*+1}^{h_*}\zeta_j^{-2}\mathrm{Var}(z_j)\mathbf{v}_j\mathbf{v}_j'\mathbf{D}'\mathbf{N}'\mathbf{r}^{-\delta}. \tag{3.26}$$

From Lemma 3.2 it follows immediately for $\mathbf{c}'\boldsymbol{\tau}$ that

$$\mathrm{E}(\widetilde{\mathbf{c}'\boldsymbol{\tau}}) = \mathbf{c}'\boldsymbol{\tau} \tag{3.27}$$

and that

$$\mathrm{Var}(\widetilde{\mathbf{c}'\boldsymbol{\tau}}) = \mathrm{Var}(\widehat{\mathbf{c}'\boldsymbol{\tau}}) + \sum_{j=g_*+1}^{h_*} \zeta_j^{-2}(\mathbf{c}'\mathbf{r}^{-\delta}\mathbf{N}\mathbf{D}\mathbf{v}_j)^2\mathrm{Var}(z_j). \tag{3.28}$$

To proceed further, it will be helpful first to note that, on account of (3.22), one can write

$$\mathbf{y}'\mathbf{R}\mathbf{G}'\mathbf{G}\mathbf{R}\mathbf{y} = \xi^{-2}n_0\sum_{j=1}^{g_*}(\mathbf{v}_j'\mathbf{y})^2, \tag{3.29}$$

$$\mathbf{y}'\mathbf{R}\mathbf{D}'\mathbf{D}\mathbf{R}\mathbf{y} = \xi^{-2}k\sum_{j=1}^{g_*}(\mathbf{v}_j'\mathbf{y})^2 + \sum_{j=g_*+1}^{h_*}\zeta_j^{-2}\lambda_j(\mathbf{v}_j'\mathbf{y})^2 \tag{3.30}$$

and

$$\mathbf{y}'\mathbf{R}\mathbf{R}\mathbf{y} = \xi^{-2}\sum_{j=1}^{g_*}(\mathbf{v}_j'\mathbf{y})^2 + \sum_{j=g_*+1}^{h_*}\zeta_j^{-2}(\mathbf{v}_j'\mathbf{y})^2 + \sum_{j=h_*+1}^{n-v}(\mathbf{v}_j'\mathbf{y})^2. \tag{3.31}$$

Thus, the estimators $\hat{\gamma}_1$ and $\hat{\gamma}_2$, as obtainable from the equations (3.10), and the random variables $\{z_j\}$, defined in (3.23) and (3.24), can be expressed as functions of $\mathbf{y}$ solely through the variables

$$x_j = \mathbf{v}_j'\mathbf{y} \qquad \text{for} \quad j = 1, ..., n-v. \tag{3.32}$$

Next, utilizing Lemma 3.3 of Caliński and Kageyama (1996a), one obtains the following result.

COROLLARY 3.1. *Let the random variables* $\{x_j\}$ *defined in* (3.32) *have mutually independent symmetric distributions around zero, in the sense that* x_j *and* $-x_j$ *are distributed identically and for each* j $(= 1, ..., n-v)$ *independently. Furthermore, let each of the statistics* $\hat{\gamma}_1$ *and* $\hat{\gamma}_2$ *be an even function of any* x_j, *in the sense that it is invariant under the change of* x_j *to* $-x_j$ *for any* j. *Then the joint distribution of the random variables* $\{z_j\}$, *defined in* (3.23) *and* (3.24), *is symmetric around zero with regard to each* z_j, *in the sense that the distribution is invariant under the change of* z_j *to* $-z_j$ *for any* j. *Hence,* $\mathrm{E}(z_j) = 0$ *for all* j *and* $\mathrm{E}(z_j z_{j'}) = 0$ *for all* $j \neq j'$ $(= 1, ..., h_*)$, *provided that these expectations exist.* [It is sufficient here to consider the random variables defined in (3.24) only.]

With these results the following main theorem (similar to Theorem 3.2 of Caliński and Kageyama, 1996a) can be proved.

THEOREM 3.2. *Let, for an NB design satisfying the conditions* (i) *and* (ii), *the observed vector* $\mathbf{y}$ *have the model* (2.1) *with properties* (2.2) *and* (2.3), *and suppose that* *the ratios* γ_1 *and* γ_2 *appearing in* (2.4) *are unknown. Furthermore, let the distribution of* $\mathbf{y}$ *be such that it induces the random variables* $\{x_j\}$ *defined in* (3.32) *to have mutually independent symmetric distributions around zero. Under these assumptions, if the statistics* $\hat{\gamma}_1$ *and* $\hat{\gamma}_2$ *used to estimate* γ_1 *and* γ_2, *respectively, are completely expressible in terms of even functions of* $\{x_j\}$, *i.e., depend on* $\mathbf{y}$ *solely through such functions, then, for all values of* γ_1 *and* γ_2 *and of their estimators satisfying the conditions* γ_1, $\hat{\gamma}_1 \geq 0$ *and* γ_2, $\hat{\gamma}_2 > -1/k_{\max}$, *the estimator* $\tilde{\boldsymbol{\tau}}$ *defined in* (3.17) *has the properties* (3.25) *and* (3.26), *and hence* $\widetilde{\mathbf{c}'\boldsymbol{\tau}}$ *has the properties as in* (3.27) *and* (3.28), *for any* $\mathbf{c}$.

This theorem can be proved in a similar way as Theorem 3.2 in Caliński and Kageyama (1996a, p.370). It should also be noted that Theorem 3.2 is general in the sense that it applies, under its assumptions, to any estimators of γ_1 and γ_2 which depend on the observed vector $\mathbf{y}$ through even functions of $\{x_j\}$ only.

Remark 3.1. In connection with the assumptions of Theorem 3.2 the following results are obtainable.

(a) The random variables $\{x_j\}$ defined in (3.32) have the properties

$$\mathrm{E}(x_j) = 0 \tag{3.33}$$

and

$$\mathrm{E}(x_j x_{j'}) = \begin{cases} \sigma_1^2 \xi & \text{for} \quad j = j' = 1, ..., g_*, \\ \sigma_1^2 \zeta_j & \text{for} \quad j = j' = g_* + 1, ..., h_*, \\ \sigma_1^2 & \text{for} \quad j = j' = h_* + 1, ..., n - v, \\ 0 & \text{for} \quad j \neq j', \end{cases} \tag{3.34}$$

resulting from the properties (2.2) and (2.4) of $\mathbf{y}$ and the definitions of the vectors $\{\mathbf{v}_j\}$.

(b) If $\mathbf{y}$ has an n-variate normal distribution, then also $\mathbf{x} = [x_1, ..., x_{n-v}]'$, with $x_j = \mathbf{v}_j'\mathbf{y}$, has an $(n-v)$-variate normal distribution, which automatically implies, on account of (3.33) and (3.34), that its elements have mutually independent symmetric distributions around zero.

(c) Since the functions of the random vector $\mathbf{y}$ appearing in equations (3.10) are, as shown in (3.29), (3.30) and (3.31), completely expressible in terms of the squares $x_j^2 = (\mathbf{v}_j'\mathbf{y})^2$, $j = 1, ..., n - v$, the statistics $\hat{\gamma}_1$ and $\hat{\gamma}_2$ obtained from the solution of these equations (or their equivalence) satisfy the conditions of Theorem 3.2, provided that their values are not below the lower limits assumed for them.

It follows from Theorem 3.2 that if the unknown values of γ_1 and γ_2 appearing in (3.3) are replaced by their estimators $\hat{\gamma}_1$ and $\hat{\gamma}_2$ obtainable in accordance with the conditions of this theorem, then the unbiasedness of the estimators of $\boldsymbol{\tau}$ and $\mathbf{c}'\boldsymbol{\tau}$ established in Theorem 3.1 is not violated (cf. Kłaczyński, Molińska and Moliński, 1994), but the variance of the estimator of $\mathbf{c}'\boldsymbol{\tau}$ is increased, as can be seen from (3.28). Although the exact formula of $\mathrm{Var}(z_j) = \mathrm{E}(z_j^2)$ is in general intractable, it can be approximated similarly as shown in Caliński and Kageyama (1996a). For this note that by expanding z_j in a Taylor series in $\hat{\gamma}$ about the point γ, where $\gamma = \gamma_1 b_0 + \gamma_2$ with $\hat{\gamma} = \hat{\gamma}_1 b_0 + \hat{\gamma}_2$ for $j = 1, ..., g_*$ and $\gamma = \gamma_2$ with $\hat{\gamma} = \hat{\gamma}_2$ for $j = g_* + 1, ..., h_*$, one obtains the approximation

$$z_j^2 \cong \left(\frac{\hat{\gamma} - \gamma}{\gamma\lambda_j + 1}\right)^2 x_j^2. \tag{3.35}$$

Then, applying Theorems 2b.3(i) and (iii) of Rao (1973) to the expectation of (3.35), one can write

$$\mathrm{E}(z_j^2) \cong \mathrm{E}\left[\left(\frac{\hat{\gamma} - \gamma}{\gamma\lambda_j + 1}\right)^2 \mathrm{E}(x_j^2 \mid \hat{\gamma})\right]. \tag{3.36}$$

If the number of x_j's from which the statistic $\hat{\gamma}$ is calculated is large, i.e., if in the case of the equations (3.10) the number $n - v$ is large, then the statistical dependence between x_j^2 and $\hat{\gamma}$ can be ignored and the unconditional expectation $\mathrm{E}(x_j^2)$ can be used instead of $\mathrm{E}(x_j^2) \mid \hat{\gamma})$. This would allow the approximation (3.36) to be replaced by

$$\mathrm{E}(z_j^2) \cong (\gamma\lambda_j + 1)^{-1}\sigma_1^2 \mathrm{E}[(\hat{\gamma} - \gamma)^2], \tag{3.37}$$

where the mean squared error $\mathrm{E}[(\hat{\gamma} - \gamma)^2]$ (MSE of $\hat{\gamma}$) becomes $\mathrm{Var}(\hat{\gamma})$ if $\hat{\gamma}$ is an unbiased estimator of γ. With the approximation (3.37), the variance (3.28) can be approximated as

$$\mathrm{Var}(\widetilde{\mathbf{c}'\boldsymbol{\tau}}) \cong \mathrm{Var}(\widehat{\mathbf{c}'\boldsymbol{\tau}}) + \sigma_1^2 \mathrm{E}[(\hat{\gamma}_2 - \gamma_2)^2] \sum_{j=g_*+1}^{h_*} \zeta_j^{-3}(\mathbf{c}'\mathbf{r}^{-\delta}\mathbf{N}\mathbf{D}\mathbf{v}_j)^2. \tag{3.38}$$

Now, to make the approximation (3.38) applicable, the MSE of $\hat{\gamma}_2$ needs evaluation or approximation. If the distribution of $\mathbf{y}$ is assumed to be normal and $\hat{\gamma}_1$ and $\hat{\gamma}_2$ are obtained by solving the equations (3.10) [or equivalently (3.14)], i.e., by the MML (REML) method, then $\mathrm{E}[(\hat{\gamma}_2 - \gamma_2)^2]$ can be replaced by the asymptotic variance of $\hat{\gamma}_2$ obtainable from the inverse of the appropriate information matrix. Noting that the information matrix associated with the MML (REML) estimation of γ_1, γ_2 and σ_1^2 is here

$$\frac{1}{2}\begin{bmatrix} \mathrm{tr}[(\mathbf{R}\mathbf{G}'\mathbf{G})^2] & \mathrm{tr}(\mathbf{R}\mathbf{G}'\mathbf{G}\mathbf{R}\mathbf{D}'\mathbf{D}) & \sigma_1^{-2}\mathrm{tr}(\mathbf{R}\mathbf{G}'\mathbf{G}) \\ \mathrm{tr}(\mathbf{R}\mathbf{D}'\mathbf{D}\mathbf{R}\mathbf{G}'\mathbf{G}) & \mathrm{tr}[(\mathbf{R}\mathbf{D}'\mathbf{D})^2] & \sigma_1^{-2}\mathrm{tr}(\mathbf{R}\mathbf{D}'\mathbf{D}) \\ \sigma_1^{-2}\mathrm{tr}(\mathbf{R}\mathbf{G}'\mathbf{G}) & \sigma_1^{-2}\mathrm{tr}(\mathbf{R}\mathbf{D}'\mathbf{D}) & \sigma_1^{-2}(n - v) \end{bmatrix}$$

(cf. Patterson and Thompson, 1971, p. 554), and taking its inverse, it can be found, on account of (3.22), that

$$\mathrm{Var}_{\mathrm{as}}(\hat{\gamma}_2) = \frac{2}{\sum_{j=g_*+1}^{h_*}(\lambda_j/\zeta_j)^2 - (n-v-a+1)^{-1}\left(\sum_{j=g_*+1}^{h_*}\lambda_j/\zeta_j\right)^2}. \tag{3.39}$$

Thus, when under the normality assumption the ratios γ_1 and γ_2 are estimated by the MML (REML) method, then the variance (3.38) can further be approximated as

$$\mathrm{Var}(\widetilde{\mathbf{c}'\boldsymbol{\tau}}) \cong \mathrm{Var}(\widetilde{\mathbf{c}'\boldsymbol{\tau}}) + \sigma_1^2 \mathrm{Var}_{\mathrm{as}}(\hat{\gamma}_2) \sum_{j=g_*+1}^{h_*} \zeta_j^{-3}(\mathbf{c}'\mathbf{r}^{-\delta}\mathbf{N}\mathbf{D}\mathbf{v}_j)^2, \tag{3.40}$$

with $\mathrm{Var}_{\mathrm{as}}(\hat{\gamma}_2)$ given in (3.39).

The approximation (3.40) is equivalent to that which has been suggested by Kackar and Harville (1984), here applied to the variance (3.28). The closeness of this approximation has not been investigated yet.

When taking into account the asymptotic properties of the MML (REML) estimators of γ_1 and γ_2, or equivalently those of the iterated MINQUE of these parameters (see, e.g., Brown, 1976; Rao and Kleffe, 1988, Chapter 10), it can be observed that, under the normality assumption, the estimators $\hat{\gamma}_1$ and $\hat{\gamma}_2$ obtained by solving the equations (3.10) [or (3.14)] are asymptotically unbiased and efficient (i.e., with the smallest possible limiting variance). Thus, it can be concluded that the approximation (3.40) approaches the exact value of $\mathrm{Var}(\widetilde{\mathbf{c}'\boldsymbol{\tau}})$ as $n-v$ tends to infinity. However, since in practical applications the increase of n over v is possible within some limits only, the formula (3.40) will always remain merely an approximation. Not much till now is known about the closeness of this approximation. It remains to be investigated.

4. Concluding remarks

The theory of estimating the vector $\boldsymbol{\tau}$ and a parametric function $\mathbf{c}'\boldsymbol{\tau}$, presented in Sections 3.1 and 3.2, is applicable to any NB design, regardless of the constructions used for the composing designs D^* and D (see Section 1). The approximation formula (3.40) for the variance of the resulting estimator of $\mathbf{c}'\boldsymbol{\tau}$ can, however, be applied under ceratin conditions only. To satisfy them it is required that the NB design is composed of a proper (equiblocksized) block design D^* and a superblock design D which is not only proper but also connected and orthogonal. These requirements are met by most NB designs commonly used in practice. Such NB designs have been considered recently by Mejza and Kageyama (1995), and called by them proper *superblock orthogonal* NB designs. Note that among the traditional block designs the well known lattice designs belong to this class of NB designs, as well as all other proper resolvable incomplete block designs (see, e.g., John, 1987, Sections 3.4 and 4.7-4.10).

In fact, the wide class of α-resolvable block designs originated by Bose (1942) and generalized by Shrikhande and Raghavarao (1963), later utilized and extended further by various authors, in particular by Kageyama (1972, 1973, 1976), by Patterson and Williams (1976), Williams (1976) and Williams et al. (1976), and by Ceranka et al. (1986), is a subclass of the above class of NB designs, with the exception of those α-resolvable block designs which are constructed as non-proper (of unequal block and/or superblock sizes). For more references on resolvable block designs see, e.g., Caliński and Kageyama (1996b, Sections 4.2 and 4.3).

It should, however, be mentioned that the most general class of resolvable block designs considered by Kageyama (1976), that which allows for unequal block and superblock sizes, exceeds the above class of NB designs. Therefore, there is still a need for an approximation formula more general than that given in (3.40). This requires some further research and is beyond the scope of the present paper.

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Odzyskiwanie informacji międzyblokowej gdy doświadczenie założone jest w układzie o blokach zagnieżdżonych

Streszczenie

W pracy omówiono ogólny model randomizacyjny dla doświadczeń planowanych w układach o blokach zagnieżdżonych (układach blokowych hierarchicznych), rozważany z punktu widzenia odzyskiwania informacji międzyblokowej. Najpierw pokazano, jak w tym modelu można otrzymać najlepsze liniowe estymatory nieobciążone funkcji liniowych parametrów obiektowych przy założeniu, że komponenty wariancyjne związane z tymi estymatorami są znane. Następnie przedstawiono ogólną metodę estymowania tych zwykle nieznanych komponentów wariancyjnych oraz podjęto próbę zbadania własności estymatorów empirycznych otrzymywanych w wyniku zastąpienia w powyższych estymatorach liniowych występujących tam komponentów wariancyjnych ich ocenami. Zaproponowano także pewną metodę aproksymowania wariancji tak uzyskiwanych estymatorów, mającą zastosowanie do większości rozważanych układów. Praca pozwala przenieść na układy o blokach zagnieżdżonych odpowiednie wyniki znane wcześniej dla zwyczajnych układów blokowych (o jednej warstwie bloków).

Słowa kluczowe: estymacja komponentów wariancyjnych, model randomizacyjny, najlepsza liniowa estymacja nieobciążona, odzyskiwanie informacji międzyblokowej, układy o blokach zagnieżdżonych (układy blokowe hierarchiczne).