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ON SOME ASPECTS OF THE OPTIMAL STATISTICAL INFERENCE ON VARIANCE COMPONENTS IN MIXED LINEAR MODELS

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I wish to dedicate this paper to the memory of Professor Stanisław Gnot—my dear friend and wonderful teacher

ABSTRACT. In the paper the problem of hypotheses testing and interval estimation for variance components in mixed linear models is considered. Mostly, the optimal statistical inference is determined by giving the uniformly most powerful (invariant or unbiased or invariant unbiased) tests (UMPIT, UMPUT or UMPIUT, respectively) or by appropriate construction of the uniformly most accurate confidence intervals (UMACI). When the UMPIT does not exist a construction of the locally best invariant unbiased test (LBIUT) for a single variance component (or for a ratio of variance components) as a basis of the optimal statistical inference is given. The major objective of this article is, on the one hand, to present strict relationships between statistical tests and confidence intervals for select functions of variance components and, on the other hand, to answer the question: whether the confidence intervals or hypotheses tests are more informative for making decisions based on parametric values? Moreover, some aspects connected with the layouts with minimal number observations that assure existence of the uniformly best unbiased estimators (UBUE) and the UMPIT for variance components are considered. The designs with different degree of data imbalance for which the optimal statistical inference based on UMPIT or UMPIUT becomes impossible, are also presented. Theoretical considerations by a simulations study for some experimental layouts are illustrated, too.

1. Introduction

We consider the general linear model

$$y = X\beta + \sum_{i=1}^{k} X_i\beta_i + e\,, \tag{1}$$

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where X, $X_1, \dots, X_k$ are known matrices, β is a p-vector of parameters corresponding to fixed effects, while $\beta_1, \dots, \beta_k$ and e are stochastically independent random vectors normally distributed with zero mean and the covariance matrix $\sigma_i^2 I_{p_i}$ $(i = 1, \dots, k)$ and $\sigma^2 I_n$, respectively. Under these assumptions we obtain

$$E(y) = X\beta, \quad \mathrm{Var}(y) = \sum_{i=1}^{k} \sigma_i^2 V_i + \sigma^2 I_n, \quad V_i = X_i X_i'. \tag{2}$$

In this paper relationships between testing hypotheses for variance components σ_i^2 or for variance ratio $\theta_i = \sigma_i^2/\sigma^2$ are presented. One can expect that tests which have desirable statistical properties lead to a "good" confidence interval. For regular models, i.e., when there exist UMPI test or UMPIU test, the UMA confidence interval also exists. However, the optimal statistical inference determined in such a way is not always desirable and profitable from the practical point of view. Hence, there emerges a need to modify an experimental design and to depart from a regular model and thus to construct a locally best invariant unbiased test or a good confidence interval. The results obtained on the base of Anderson's and Wijsman's approach are related to a representation of maximal invariant density and based on generalized Neyman–Pearson's Lemma.

2. Testing hypothesis for $\theta_i = \sigma_i^2/\sigma^2$

In the problem of invariant estimation of variance components we can choose a maximal invariant determined by $t_M = My$: $M = I - XX^+$ or in the form of $t = By$: $BB' = I_{n-p}$, $B'B = I - XX^+$. This choice has no influence on the value of the optimal estimator, and properties of the considered model may be presented both in terms of the subspace $\mathcal{V}_M = \mathrm{sp}\{MV_1M, \dots, MV_kM, M\}$ and of the subspace $\mathcal{V} = \mathrm{sp}\{BV_1B', \dots, BV_kB', I_{n-p}\}$, respectively. By Seely's (1971) theorem, the statistical properties of the general linear model ensuring the existence of an uniformly best unbiased estimator of each estimable function $f'\sigma$ for $\sigma = (\sigma_1^2, \dots \sigma_k^2, \sigma^2)$ depend on the algebraic properties of the subspace $\mathcal{V}_M$ or those of the subspace $\mathcal{V}$, equivalently. Therefore, it is clear, that in the general linear model for each quadratically and invariantly estimable function there exists an uniformly best unbiased and invariant estimator if and only if the supspace $\mathcal{V} = \mathrm{sp}\{BV_1B', \dots, BV_kB', I_{n-p}\}$ is a Jordan algebra, or equivalently $\mathcal{V}$ is quadratic subspace.

Note. The model satisfying such a condition is called a regular model.

Now, we are interested in interval estimation of the variance ratio $\theta_i = \sigma_i^2/\sigma^2$, where $[0, \infty)$ defines a natural space for the parameter θ_i. This problem is strictly connected with testing of the hypothesis

$$H\colon \theta_i = 0 \quad \text{vs} \quad K\colon \theta_i > 0 \tag{3}$$

or more general

$$H_*\colon \theta_i = \theta_0 \quad \text{vs} \quad K_*^+\colon \theta_i > \theta_0 \quad (K_*^-\colon \theta_i < \theta_0) \tag{4}$$

or for two-sided alternatives

$$H_*\colon \theta_i = \theta_0 \quad \text{vs} \quad K_*\colon \theta_i \neq \theta_0 \,. \tag{5}$$

We construct tests for hypothesis (4) or (5) on the basis of the following alternative approaches: the modification of Wald's idea, the decomposition of quadratic form of an unbiased invariant estimator of σ_i^2 and using the distribution of maximal invariant with Neyman–Pearson's idea. All obtained tests are invariant under the group $\mathcal{G}$ of transformations $y \mapsto c(y + X\beta)$, $c > 0$, $\beta \in \mathbb{R}^p$ and the reduction by invariance principle leads to a ratio test statistics.

The test based on the modification of Wald's idea has been proposed, in models with two variance components, by Gnot and Michalski (see 1991, 1994). The construction of this test combines algebraic premises with statistical properties of estimators of function $\rho_{\max}\sigma_i^2 + \sigma^2$ (for some optimal choice $\rho_{\max}$) and σ^2, which occur in a ratio statistic, in the numerator and in the denominator, respectively (see Section 3). We can extend our construction of the test for hypothesis (4) on the general linear model assuming the matrices V_i are linearly independent and using some results concerning admissible estimators of functions $f'\sigma$ (see LaMotte (1982), Gnot (1983, 1991), Klonecki and Zontek (1988) and also Gnot *et al.* (1992)).

The second approach introduced by Michalski and Zmyślony (1996) requires the assumption that there exists a smallest commutative quadratic subspace generated by $\mathcal{V}$ with orthogonal projections $E_1, \ldots, E_k, E_{k+1}$ which form its base. Next, for an invariant unbiased estimator of settled component σ_i^2, $i = 1, \ldots, k$ in form $y'Ay$, we perform a decomposition of this quadratic form into the positive and the negative part, i.e., $A_+ = \sum_{j\in\mathcal{K}_1} c_j E_j$ and $A_- = \sum_{j\in\mathcal{K}_2} c_j E_j$, where $\mathcal{K}_1 = \{j\colon c_j > 0\}$ and $\mathcal{K}_2 = \{j\colon c_j < 0\}$ are disjoint subsets of $\{1, \ldots, k, k+1\}$ which in turn implies that $A_+A_- = 0$. Finally, the test statistic is built as the ratio $F = y'A_+y/y'A_-y$.

Note. It is interesting that this method allows to gain a lot of known results from classic mathematical statistics (see Michalski and Zmyślony (1999), Gąsiorek *et al.* (2000)).

The last approach is based on the Wijsman's Representation Theorem (cf. Wijsman (1967), King (1980, Theorem 1)) which concerns the probability ratio $R(T(y))$ of maximal invariant $T(y)$ (here $T(y) = By$) under group $\mathcal{G}$.

Using the (generalized) Neyman–Pearson Lemma to obtain the test statistic we examine the ratio R of density functions of T under the alternative $K_*: \theta_i = \theta_*$ and under null hypothesis $H_*: \theta_i = \theta_0$ (cf. M a t h e w (1988) and K h u r i *et al.* (1998)); see also Section 3 and 4.

3. Two variance components model

Assuming in this section that $k = 1$, the variance-covariance matrix of our model reduces to $\sigma^2(\theta V_1 + I_n)$, $V_1 = X_1 X_1'$. It is easy to check that the quadratic subspace $\mathcal{V} = \{BV_1B',\ I_{n-p}\}$ is commutative (cf. G n o t and K l e f f e (1983)) and we can construct an exact test for hypotheses (4) or (5). Let $\alpha_1 > \alpha_2 > \cdots > \alpha_{h-1} > \alpha_h = 0$ be the ordered sequence of different eigenvalues of $W = BV_1B'$ with multiplicity $\nu_1, \ldots, \nu_{h-1}, \nu_h$, respectively. Thus, we have

$$W = BV_1B' = \sum_{j=1}^{h} \alpha_j E_j \qquad \text{and} \qquad \mathcal{V} = \mathrm{sp}\{E_1, \ldots, E_{h-1}, E_h\},$$

$$\text{where} \quad E_h = I_{n-p} - \sum_{j=1}^{h-1} E_j \quad \text{with} \quad \mathrm{trace}(E_j) = \nu_j .$$

3.1 Maximal invariant statistics

Following O l s e n *et al.* (1976) the minimal sufficient statistics for the family of distributions of a maximal invariant statistics $t = By$ under the group $\mathcal{G}$ are formed by quadratic forms $Z_i = t'E_it/\nu_i$, for $i = 1, \ldots, h-1, h$, which are stochastically independent. Moreover, the variables $\nu_i Z_i / \big(\sigma^2(\theta_i \alpha_i + 1)\big)$ are centrally chi-square distributed with ν_i degrees of freedom, $i = 1, \ldots, h$. The model for $Z = (Z_1, \ldots, Z_{h-1}, Z_h)$ is as follows

$$\begin{cases} E(Z) = L(\sigma_1^2, \sigma^2)'; \quad L' = \begin{bmatrix} \alpha_1 & \ldots & \alpha_h \\ 1 & \ldots & 1 \end{bmatrix} \\ \mathrm{Var}(Z) = 2\,\mathrm{diag}\big\{(\alpha_1\sigma_1^2 + \sigma^2)^2/\nu_1, \ldots, (\alpha_h\sigma_1^2 + \sigma^2)^2/\nu_h\big\}. \end{cases} \tag{6}$$

A maximal invariant statistics with respect to group transformations $\mathcal{G}$ is

$$Z_0 = (Z_1/Z_h, \ldots, Z_{h-1}/Z_h)'.$$

It has been established by T h o m p s o n (1955) and M a t h e w (1989) that the density function of Z_0 is proportional to

$$\left[1 + \sum_{i=1}^{h-1} \frac{\nu_i Z_i}{\nu_h Z_h (1 + \alpha_i \theta)}\right]^{-r/2}, \qquad r = \mathrm{rank}(W). \tag{7}$$

3.2 Review of the invariant tests

The problem of testing the hypothesis (3) has been considered by several authors. A review of invariant tests can be find in Gnot *et al.* (1992) (see also Michalski 2000). Some of them based on the maximal invariant statistics Z_0 for the hypothesis (3) or (4) are presented below.

Wald's test (Seely and El-Bassiouni 1983). The test is based on the statistic

$$F_{\mathbf{W}} = \frac{\sum_{i=1}^{h-1} \nu_i Z_i}{\nu_h Z_h} = \frac{y'\Pi_1 y}{y'\Pi_2 y},$$

where Π_1 and Π_2 are the orthogonal projectors on $\mathcal{R}(X \vdots X_1) \cap \mathcal{N}(X')$ and $\mathcal{N}(X') \cap \mathcal{N}(X_1')$, respectively. Here for an arbitrary matrix A the symbol $\mathcal{R}(A)$ stands for range (image) of A and the symbol $\mathcal{N}(A)$ denotes the kernel of A.

Modified Wald's test (cf. Gnot and Michalski 1991, 1994). The test is based on

$$F_{\mathbf{W}}^* = \begin{cases} \sum_{i=1}^{h} (\alpha_i - \alpha_h)\nu_i Z_i / \sum_{i=1}^{h} (\alpha_1 - \alpha_i)\alpha_i^{-2}\nu_i Z_i & \text{for } \alpha_h > 0, \\ \sum_{i=1}^{h-1} \alpha_i \nu_i Z_i / \nu_h Z_h & \text{for } \alpha_h = 0. \end{cases}$$

Note. The case $\alpha_h > 0$ means that the variance-covariance matrix W is nonsingular and in these situations the construction based on Wald's idea is impossible. These cases appear in an experimental designs with minimal number of observations and will be considered in Section 4. The numerator of F_W^* ratio in both cases represents the statistic which is proportional to the unique admissible estimator of the function $\rho_{\max}\sigma_1^2 + \sigma^2$, where $\rho_{\max} = \operatorname{trace}(W^2)/\operatorname{trace}(W)$.

Neyman–Pearson's test (cf. Thompson 1955, LaMotte *et al.* 1988, Westfall 1989). The test is obtained from the Neyman–Pearson's lemma. For testing $H\colon \theta = \theta_0$ vs $K_*\colon \theta = \theta_*$ $(\theta_* \neq \theta_0)$ the test statistic is

$$F_{\mathbf{NP}}(\theta_0, \theta_*) = \frac{\sum_{i=1}^{h} \nu_i Z_i/(1 + \alpha_i\theta_0)}{\sum_{i=1}^{h} \nu_i Z_i/(1 + \alpha_i\theta_*)}.$$

Locally best invariant test. (Das and Sinha 1987, Mathew and Sinha 1988). The test statistic is obtained as a result of maximization of the density function (7) at $\theta = 0$ i.e., in a small right-hand neighbourhood of the null hypothesis. It is as follows

$$F_{\mathbf{LB}} = \frac{\sum_{i=1}^{h-1} \alpha_i \nu_i Z_i}{\sum_{i=1}^{h} \nu_i Z_i}.$$

LM test. (L a M o t t e *et al.* 1988). The test statistic has the form

$$F_{\mathbf{LM}} = \frac{\sum_{i=d+1}^{h} \nu_i Z_i}{\sum_{i=1}^{d} \nu_i Z_i},$$

where d is an arbitrary integer from $(1, h)$ which gives such division of statistics Z_i to obtain the test on the maximal power.

$\mathbf{A}_{-}^{+}$ **test** (M i c h a l s k i and Z m y ś l o n y 1996). The test is based on the statistic

$$F_{\mathbf{A}_{-}^{+}} = \frac{y' A_+ y}{y' A_- y} = \frac{\sum_{\alpha_i^* > 0} \nu_i \alpha_i^* Z_i}{-\sum_{\alpha_i^* < 0} \nu_i \alpha_i^* Z_i},$$

obtained from the decomposition $A = A_+ - A_-$ into the positive and the negative parts of the matrix A such that $y'Ay$ is MINQUE for σ_1^2. Here $\alpha_i^* = \alpha_i - \operatorname{trace}(W)/\operatorname{rank}(W)$.

Note. The preceding test has been constructed using the Bayes locally best unbiased quadratic invariant estimator of σ_1^2 at the point $(\sigma_1^*, \sigma^*) = (0, 1)$. For the modified Wald's test as well as for the above test having the prior distribution on (σ_1^2, σ^2) we can obtain an optimal test for hypothesis (4) or (5).

The hypothesis $H\,(H_*)$ against alternatives $K\,(K_*^+)$ is rejected for large (small, vs K_*^-) values of the test statistics.

Remark 3.1. In the case $h = 2$ all tests under study are equivalent except for the case $\alpha_2 > 0$ (W is nonsingular) when the Wald's test does not exist.

3.3 Exact confidence intervals

In this section we present strict relationships between tests and confidence intervals for the variance ratio $\theta_i = \sigma_i^2/\sigma^2$. Each of the test statistics presented above for the problem of testing hypotheses (3) or (4) can be used to construct exact confidence intervals of θ_i.

The case $h = 2$**.** In this case (see Remark 3.1) we can construct exact confidence intervals using the invariant maximal statistic $Z_0 = Z_1/Z_2$ as in the following theorem.

THEOREM 3.1. (Michalski 1995) *There exists the uniformly most accurate unbiased* (UMAU) $1-p$ *confidence interval on* θ *in the model* (2), *for* $k=1$ *iff the number* h *of the different eigenvalues* α_i *with multiplicity* ν_i *of the covariance matrix* W *is 2. Then the confidence interval for* θ *has the following form*

$$\frac{1}{\alpha_1}\left[\frac{Z_0-\phi^{-1}(1-p_2)}{\phi^{-1}(1-p_2)-Z_0\alpha_2/\alpha_1};\ \frac{Z_0-\phi^{-1}(p_1)}{\phi^{-1}(p_1)-Z_0\alpha_2/\alpha_1}\right], \tag{8}$$

where $Z_0 = Z_1/Z_2$, p_1 *and* p_2 *are arbitrary positive scalars such that* $p_1+p_2 = p$, *while* $\phi(\cdot)$ *denotes the cumulative density function of the* F*-distribution with* ν_1 *and* ν_2 *degrees of freedom.*

The general case ($h > 2$)**.** If $h>2$ then the UMAU $1-p$ confidence interval does not exist and in this case the construction of $1-p$ confidence intervals on θ may be based on several test statistics presented in Section 3.2. In general, if we have a satisfactory test for a single parameter θ, we also have a reliable confidence interval for this parameter. Now, we propose the construction of exact confidence intervals for the ratio θ based, e.g., on statistics $F^*_{\mathbf{W}}$ (or $F_{\mathbf{NP}}(\theta,\theta_0,\theta_*)$). By some scale transformation of Z each test statistics ϕ corresponds to a function $G_\phi(\theta)$ of the parameter θ such that for fixed θ we know its probability distribution. And so, for the statistics $F^*_{\mathbf{W}}$ we have

$$G_{W^*}(\theta) = \frac{\sum_{i=1}^{h-1}\alpha_i\nu_i Z_i/(1+\alpha_i\theta)}{\nu_h Z_h}, \tag{9}$$

and for the statistics $F_{\mathbf{NP}}(\theta_0,\theta_*)$ we obtain

$$G_{\mathbf{NP}}(\theta,\theta_0,\theta_*) = \frac{\sum_{i=1}^{h}\nu_i Z_i/(1+\alpha_i\theta)/(1+\alpha_i\theta_0)}{\sum_{i=1}^{h}\nu_i Z_i/(1+\alpha_i\theta)/(1+\alpha_i\theta_*)}, \tag{10}$$

where fixed θ_0 and θ_* are connected with null and alternative hypothesis described by (4) or (5), respectively.

It is easy to show that $G_\phi(\theta)$ for given test statistic ϕ is a strictly convex and decreasing function of $\theta \in [-1/\alpha_1,\infty)$. The distribution of $G_\phi(\theta)$ is the same as the distribution of the ratio of positive linear combinations of independent central chi-squared random variables in general form

$$\frac{\sum_{i=1}^{h} w_i \chi^2_{\nu_i}}{\sum_{i=1}^{h} w'_i \chi^2_{\nu_i}} .$$

Now, in order to construct the $1-p$ confidence intervals $(p_1+p_2=p)$ we must find the critical values C_{p_1} and C_{p_2} such that

$$\Pr\left\{ C_{p_1} \le \frac{\sum_{i=1}^{h} w_i \chi^2_{\nu_i}}{\sum_{i=1}^{h} w'_i \chi^2_{\nu_i}} \le C_{p_2} \right\} = 1 - p_1 - p_2 \tag{11}$$

or, equivalently,

$$\begin{cases} \Pr\left\{ \sum_{i=1}^{h} (w_i - C_{p_1} w'_i) \chi^2_{\nu_i} > 0 \right\} = 1 - p_1 , \\ \Pr\left\{ \sum_{i=1}^{h} (C_{p_2} w'_i - w_i) \chi^2_{\nu_i} > 0 \right\} = p_2 . \end{cases} \tag{12}$$

Thus the solutions C_{p_1} and C_{p_2} of (11) or (12) are based on the distribution of quadratic forms $Q = \sum_{i=1}^{m} \lambda_i \chi^2_{\nu_i}$ (for details see, e.g., Imhof 1961, Davies 1980). Next, we must solve two following nonlinear equations

$$G_\phi(\bar{\theta}) = C_{p_1} \qquad \text{and} \qquad G_\phi(\underline{\theta}) = C_{p_2} , \tag{13}$$

where $G_\phi(\theta)$ is determined by (9) or (10) and $0 < C_{p_1}, \ C_{p_2} \le G_\phi(0)$. The solution is ensured by the properties of $G_\phi(\theta)$. In consequence of (13) we obtain the following form of the $1-p$ confidence interval of the parameter θ

$$[\underline{\theta}, \overline{\theta}] = \left[G^{-1}_\phi(C_{p_2}), G^{-1}_\phi(C_{p_1}) \right] .$$

Finally, the problem arises how to allocate $p = p_1 + p_2$, such that the probability in the left tail is p_1 and the probability in the right tail is p_2. For this purpose it seems to be optimal to choose a pair (p_1^0, p_2^0) so as to minimize the length $l(p_1, p_2)$ of the $1-(p_1+p_2)$ confidence interval, i.e.,

$$l(p_1^0, p_2^0) = \min_{\substack{p_1, p_2 \\ p_1 + p_2 = p}} \left[G^{-1}_\phi(C_{p_1}) - G^{-1}_\phi(C_{p_2}) \right] .$$

Remark 3.2. It should be noted that there are interesting relations between the statistics, and so, $\lim_{\theta_* \to \theta_0} F_{\mathbf{NP}}(\theta_0, \theta_*) = F_{\mathbf{LB}}$, $\lim_{\theta_* \to \infty} F_{\mathbf{NP}}(\theta_0, \theta_*) = F_{\mathbf{W}}$

(cf. Westfall 1989, Lin and Harville 1991). Moreover, in graphic interpretation the functions $G_{\mathbf{NP}}(\theta, \theta_*)$ form a characteristic surface of hyperboles with asymptotes at point $-1/\alpha_1$ (a hyperbolic cone) with upper hyperbolic function connected with statistic $F_{\mathbf{W}}$ and lower limit $G(\theta) = \text{const} = 1$, the function $G_{\mathbf{LB}}(\theta)$ corresponding to the test statistic $F_{\mathbf{LB}}$ describes hyperbole situated below 1.

The test statistics $F^*_{\mathbf{W}}$ and $F_{\mathbf{A}^+_-}$ in general case depend on the prior distribution on (σ_1^2, σ^2) described by the pair of parameters (u, v), $u \geq 0$, $v \geq 0$, and in fact we have the whole class tests. The functions $G^*_{\mathbf{W}}(\theta)$ or $G_{\mathbf{A}^+_-}(\theta)$ corresponding to the proper test statistics $F^*_{\mathbf{W}}$ and $F_{\mathbf{A}^+_-}$ form some specific hyperbolic cones. The facts indicate a rich choice of test statistics for the construction of a reliable confidence interval at a fixed confidence level. For details we refer to paper of Michalski (2000).

4. Regular models

Because of strong algebraic restrictions ($\mathcal{V}$ forms a quadratic subspace) in regular models the structure of the variance-covariance matrix is not very complicated. Full characteristic of regular models is not known. A wide class of the models was given by Searle and Henderson (1979). For these models matrices X and V_i can be presented as Kronecker products of identity matrix I and matrices composed of numbers equal 1, i.e., in the form $\mathbf{1}\mathbf{1}'$, $\mathbf{1} = (1, \ldots, 1)'$. The models of more complicated structure of covariance matrix are mainly connected with block designs. Seely (1977) proved that if the model is regular then in case of normal distribution of the observation vector y there exists a sufficient and complete statistic such that UBI estimators are functions of this statistic. This means that the UBI estimators are best in the class of all unbiased and invariant estimators (cf. Zmyślony 1980). The regular models corresponding to experimental designs not always ensure reliable statistical inference on parameters of model as for example for two-way layouts treated below.

4.1 Layouts with the minimal number of observations

Let us consider an experiment in which n experimental units are arranged in v rows and b columns according to the $(v \times b)$ incidence matrix N with entries $n_{ij} \geq 0$. It is assumed that the linear model corresponding to the two-way layouts described above is the mixed model with random row effects, with fixed column effects and without interaction. It can be presented as

$$y = X\beta + U\xi + e\,, \tag{14}$$

where y is a $(n \times 1)$ vector of observations, β is a $(b \times 1)$ vector of unknown column effects, ξ is a $(v \times 1)$ vector of random row effects with the expectation 0 and covariance matrix $\sigma_1^2 I_v$, while e is a $(n \times 1)$ vector of errors with the expectation 0, covariance matrix $\sigma^2 I_n$ and uncorrelated with ξ. Besides X and U are $(n \times b)$ and $(n \times v)$ known $(0,1)$-matrices of full ranks b and v. It is clear that $U'X = N, U'U = D_r$ and $X'X = D_c$, where D_r and D_c are diagonal matrices with the diagonal elements being the components of $r = N\mathbf{1}_b$ and $\kappa = N'\mathbf{1}_v$, respectively. Under these assumptions the model (14) has the following probabilistic structure

$$E(y) = X\beta\,, \quad \mathrm{Coy}(y) = \sigma_1^2 UU' + \sigma^2 I_n\,. \tag{15}$$

For the model (14) we have $\mathcal{V}_M = \{MD_rM, M\}$ and $\mathcal{V} = \{BD_rB', I_{n-p}\}$, where $M = I_n - XD_c^{-1}X' = B'B$. Let us consider the $(v \times v)$ matrix C, associated with design, as follows

$$C = D_r - ND_c^{-1}N'\,.$$

Since $C\mathbf{1}_v = \mathbf{0}_v$ (vector of zero's), $\mathrm{rank}(C) \leq v-1$. Let $\mathrm{rank}(C) = v - q$, $1 \leq q \leq v-1$. If $q = 1$ then the layout is called connected, for $q > 1$ the layout is said to be $q-$disconnected. It has been proved by K a g e y a m a (1985) that

$$n \geq v + b - q\,.$$

Thus $n = v+b-q$ is the minimal number of observations for the two-way layout with $\mathrm{rank}(C) = v-q$. If $n > v+b-1$, then $\nu_h = n-v-b+1$ is the multiplicity of the zero eigenvalues of the covariance matrix $W = BD_rB'$.

Example 1.

$$N = \begin{bmatrix} 1 & & & & \\ & \cdot & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & 1 \\ 1 & \cdot & \cdot & \cdot & 1 \end{bmatrix} = \begin{bmatrix} I_{v-1} \\ --- \\ \mathbf{1}'_{v-1} \end{bmatrix}, \tag{16}$$

$n = v+b-1$, the matrix W is nonsingular and $\alpha_1 = v/2$ with $\nu_1 = 1$, $\alpha_2 = 1/2$ with $\nu_2 = v-2$.

The class consisting of layouts with the incidence matrices isomorphic, with respect to permutations of rows and/or columns, to N given by (16) has been considered by B a k s a l a r y *et al.* (1990). According to Theorem 3 from this paper, when $v \geq 3$ and N given by (16) then under corresponding mixed model (14) there exist the UBIQU estimator for every function $f_1\sigma_1^2 + f_2\sigma^2$. The above model also assures the existence of the UMPIT for testing (3) (see G n o t *et al.* 1992, Lemma 2.2). It follows from Lemma 3.2 in M i c h a l s k i and

Srzednicka (1993) that the power function $p_\phi(\theta)$ of the UMPIT at level p for testing (3) does not achieve 1 even for limiting alternatives. The table below shows $\lim_{\theta\to\infty} p_\phi(\theta)$ as a function of v for layouts with the incidence matrix having the structure described by (16); (the sig. level $p = 0.05$).

v	3	5	10	16	20	50	200	500	1000
$p_\phi(\infty)$	.0862	.2498	.4867	.6002	.6441	.7774	.8892	.9300	.9505

Moreover, numerous examples from simulation studies (see Michalski and Srzednicka 1993) show that also the variance of UBIQUE is significantly greater than the variance of estimators in similar models (i.e., characteristics of experimental designs: v, b, n are the same) but where UBIQUE does not exist.

We can obtain better statistical properties by some modification of these designs, but standing also in the class of regular models. This needs an increase of the number of observations. The effective modification consists in adding the columns $(1, \dots 1, 0)$ to the incidence matrix N as in Example 2, presented below.

Example 2. Let us consider the layouts for which the associated matrix C has the following form

$$C = \eta(I_v - \mathbf{11}'/v).$$

This design is called variance balanced design. In the case that the matrix W has two different eigenvalues, namely $\alpha_1 = \eta = v/2$ with $\nu_1 = v - 1$; $\alpha_2 = 0$ with $\nu_2 = n - v - b + 1$, the UMPIT exists.

Now, for the particular example, we consider the design in terms of incidence matrix N

$$N = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 \end{bmatrix} ; \quad v = 5, \quad b = 6, \quad n = 16.$$

Below the values of power function $p(\theta)$ of the UMPI test are presented

θ	.001	.01	.1	.5	1	5	10	50	100	500	∞
$p(\theta)$	.0503	.0526	.0782	.2114	.3693	.8448	.9436	.9968	.9992	.9999	1

As we can see the behaviour of the power function has changed a lot. It goes to 1 very fast when θ tends to infinity.

5. Irregular models

In this section we consider models for which the statistical inference is not unique and where there is a rich choice of the decision functions. These models will be called irregular.

5.1 Layouts with the minimal number of observations

EXAMPLE 3. Layouts with the incidence matrices N described below have been examined and characterized by Kageyama (1985). It is interesting to note that for these designs the information in the matrix N columnwise increases, but the design remains connected. The covariance matrix W is the same as in Example 1. Being also nonsingular its number h of different eigenvalues is greater than 2. Hence in this case the UMPIT does not exist.

$$N = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}; \quad v = 11, \quad b = 4, \quad n = v + b - 1 = 14\,.$$

i	1	2	3	4	5	6	7
α_i	1.89	1.67	1.43	1.00	0.57	0.33	0.11
ν_i	1	1	1	4	1	1	1

The table below shows the values of the power functions $p_\phi(\theta)$ of tests ϕ based on the statistics: $F_{\mathbf{NP}}(\theta_*)$, $\theta_* = 0.1$, $F_{\mathbf{LB}}$, $F^*_{\mathbf{W}}$, $F_{\mathbf{A}^+_-}$, respectively. In the last column of the table the attainable upper bounds (AUB) of the power functions are presented. The values of AUB have been defined by LaMotte *et al.* (1988) as values of the power function of the NP test at each point $\theta = \theta_*$. The powers of the tests have been computed using a modified procedure of Imhof (1961), (see also Michalski 1990).

The inspection of this table shows a low level of power functions of all the tests even for very far alternatives. For examples 1 and 2 there do not exist tests with Wald structure, the covariance matrix W is positively definite and

θ	$p_{\mathbf{NP}}$	$p_{\mathbf{LB}}$	$p_{\mathbf{W}^*}$	$p_{\mathbf{A}^{\pm}}$	AUB
.010	.0511	.0511	.0508	.0507	.0511
.050	.0556	.0556	.0538	.0535	.0556
.100	.0610	.0610	.0574	.0569	.0610
.500	.0987	.0981	.0836	.0789	.0988
1.000	.1344	.1316	.1100	.0980	.1344
5.000	.2290	.2251	.2138	.1507	.2540
10.000	.2582	.2530	.2619	.1666	.3013
50.000	.2890	.2822	.3308	.1834	.3638
100.000	.2934	.2864	.3433	.1859	.3746
500.000	.2974	.2899	.3541	.1879	.3840
1000.000	.2996	.2918	.3581	.1898	.3915

it is worth to note the influence of the zero eigenvaules on the quality of the statistical inference (see Example 2).

The fact that the power function of the test for testing (3) is essentially less than one even for far alternatives makes the layouts with the minimal number of observations unacceptable for practice if mixed models are assumed. Now we demonstrate a way to modify the experimental designs described in Example 1 by departing from the regular model, but saving all the characteristics of the design with minimal number of observations. As competing designs let us consider q-disconnected layouts with the incidence matrix $N^{(q)}$ having the form

$$N^{(q)} = \begin{bmatrix} I_{v-q} & \vdots & \\ -- & & \mathbf{0} \\ \mathbf{1}'_{v-q} & \vdots & \\ -- & & -- \\ \mathbf{0} & \vdots & 2I_{q-1} \end{bmatrix}, \quad 1 < q \leq v-1. \tag{17}$$

Comparing (16) and (17) we see that the number of observations as well as the numbers of levels of two factors for both layouts are the same. However, in the model corresponding to layout with the incidence matrix (17) the covariance matrix W is now singular and has three different eigenvalues $\alpha_1 = (v-q+1)/2$ with $\nu_1 = 1$, $\alpha_2 = 1/2$ with $\nu_2 = v-q-1$ and $\alpha_3 = 0$ with $\nu_3 = q-1$.

The modification of the design runs in the following direction

$$N \Rightarrow N^{(2)} \Rightarrow \cdots \Rightarrow N^{(v-2)} = \begin{bmatrix} 1 & 0 & \vdots & \\ 0 & 1 & \vdots & \mathbf{0} \\ 1 & 1 & \vdots & \\ - & - & & -- \\ & \mathbf{0} & \vdots & 2I_{v-3} \end{bmatrix} \Rightarrow N^{(v-1)} = \begin{bmatrix} \mathbf{1}_2 & \vdots & \mathbf{0} \\ - & & --- \\ \mathbf{0} & \vdots & 2I_{v-2} \end{bmatrix}.$$

It has been examined (see Michalski and Srzednicka 1993) that the behaviour of the power function of the locally best test in the model with $N^{(q)}$ is quite different than in the case when UMPIT exists (regular model). The functions tend to 1 very fast if θ tends to infinity.

5.2 Construction of the LBIU test

Various practical situations and numerous examples (see Section 4) indicate that often it is better to depart from regular model and to perform the statistical inference on the basis of the locally best estimators or tests in the class with some statistical properties. In this section we give a method of the locally optimal statistical inference when we have additional information about interesting parameter of the examined model.

Let us consider the underlying testing problem in two variance component model (Section 3) as follows:

$$H_*: \theta = \theta_0 \quad \text{vs} \quad K_*: \theta = \theta_* \quad (\theta_* \neq \theta_0). \tag{18}$$

The problem of testing is invariant with respect to group transformations $\mathcal{G}$ and for the maximal invariant statistic $t = By$, B is the matrix defined in the Section 2, density function $f(t, \theta)$ has the form

$$f(t,\theta) = C\,|\Sigma|^{-1/2}(\nu_h Z_h)^{r/2}\left[\sum_{i=1}^{h} \frac{\nu_i Z_i}{1+\alpha_i\theta}\right]^{-r/2}, \tag{19}$$

where C is a some constant, $|\cdot|$ denotes the determinant, $r = \mathrm{rank}(W)$. If w is a critical region such that $\int_w f(t, \theta \mid \theta = \theta_0)\,d\mu(t) = p$ then the power function of the test is

$$p(\theta) = \int_w f(x,\theta)\,d\mu(x)\,,$$

where μ stands for the Lebesgue measure on $\mathbb{R}$ and p is a fixed significance level of a test.

Let $p(\theta)$ admit Taylor expansion around a point $\theta = \theta_0$, namely

$$p(\theta) = p(\theta_0) + (\theta-\theta_0)p'(\theta_0) + \frac{(\theta-\theta_0)^2}{2!}p''(\theta_0) + \ldots\,,$$

where $p(\theta_0) = p$ and $p'(\cdot)$, $p''(\cdot)$ denote the first and the second derivative of function $p(\cdot)$, respectively. Next, we assume that the density function $f(t,\theta)$ is regular, in the sense, that it is differentiable with respect θ and the differentiation with the integration is commutative.

Then, on the basis of the generalized Neyman–Pearson's Lemma the optimal critical region for the locally best invariant unbiased test (LBIUT) is given as

$$w_0 = \left\{ t \colon \frac{f''(t,\theta_0)}{f(t,\theta_0)} \geq k_1 \frac{f'(t,\theta_0)}{f(t,\theta_0)} + k_2 \right\}, \tag{20}$$

for $f(t,\theta)$ described by (19) and for the numbers k_1, k_2 for which the region w_0 satisfies the following conditions

$$\begin{cases} p(\theta_0) = \int\limits_{w_0} f(x,\theta_0)\, d\mu(x) = p\,, \\ p'(\theta_0) = \int\limits_{w_0} f'(x,\theta_0)\, d\mu(x) = 0 \end{cases} \tag{21}$$

(cf. R a o 1973, pp. 446–448).

Remark 5.1. The optimal region w_0 given by (20) realizes a maximum

$$p''(\theta_0) = \int\limits_{w_0} f''(x,\theta_0)\, d\mu(x)\,.$$

Equivalently, the LBIU test can be determined using Anderson's and Wijsman's representation of the probability ratio $R(T(t))$ of the maximal invariant $T = t/\parallel t \parallel$, $t = By$, while $\parallel t \parallel = \sqrt{t't}$. The ratio R of the density function of T under alternative $H_* \colon \theta = \theta_*$ and under the null hypothesis $H_0 \colon \theta = \theta_0$ has the following form

$$R = \frac{\left|\Sigma(\theta_0)\right|^{1/2}}{\left|\Sigma(\theta_*)\right|^{1/2}} \frac{\left|X'\Sigma(\theta_0)X\right|^{1/2}}{\left|X'\Sigma(\theta_*)X\right|^{1/2}} \left[\frac{t'(I+\theta_* W)^{-1}t}{t'(I+\theta_0 W)^{-1}t}\right]^{-r/2},$$

where $\Sigma(\theta) = I + \theta W$ and the spectral decomposition $W = \sum\limits_{i=1}^{h} \alpha_i E_i$ (cf. M a t h e w 1988, K h u r i *et al.* 1998).

Finally, the test statistic based on the Neyman–Pearson's Lemma for hypotheses testing (18) has the form given by

$$NP(\theta_0,\theta_*,t) = \frac{t'(I+\theta_0 W)^{-1}t}{t'(I+\theta_* W)^{-1}t} = \frac{\sum\limits_{i=1}^{h} \nu_i Z_i/(1+\alpha_i\theta_0)}{\sum\limits_{i=1}^{h} \nu_i Z_i/(1+\alpha_i\theta_*)}\,. \tag{22}$$

THEOREM 5.1. *The* LBIU *test for testing two-sided hypotheses determined by* (5) *at fixed significance level* p *has the following form*

$$\phi(t) = \begin{cases} 1, & NP(\theta_0, \theta_0, t) > C_{p_1} \ \ \textit{or} \ \ NP(\theta_0, \theta_0, t) < C_{p_2}, \\ 0, & \textit{else}, \end{cases} \tag{23}$$

where the test statistic $NP(\theta_0, \theta_0, t)$ *is given by*

$$NP(\theta_0, \theta_0, t) = \frac{\sum_{i=1}^{h} \nu_i Z_i/(1+\alpha_i\theta_0)^2}{\sum_{i=1}^{h} \nu_i Z_i/(1+\alpha_i\theta_0)}$$

and the critical values C_{p_1}, C_{p_2} *assure a fixed significance level* $p = p_1 + p_2$.

P r o o f . Let us consider the test statistic defined by (22) for testing of simple hypotheses (18) and let us examine the behaviour of this statistic when the alternatives θ_* tend to the null hypothesis θ_0, i.e., $\lim_{\theta_* \to \theta_0^+} NP(\theta_0, \theta_*, t)$ and $\lim_{\theta_* \to \theta_0^-} NP(\theta_0, \theta_*, t)$. Hence, we obtain the optimal critical region w_0 as follows

$$w_0 = \left\{t \colon NP(\theta_0, \theta_0, t) > C_{p_1} \text{ or } NP(\theta_0, \theta_0, t) < C_{p_2}\right\},$$

where $NP(\theta_0, \theta_0, t) = \lim_{\|\theta_* - \theta_0\| \to 0} NP(\theta_0, \theta_*, t)$. By straightforward calculations for $\theta_* > \theta_0$ we have

$$\frac{\sum_{i=1}^{h} \nu_i Z_i/(1+\alpha_i\theta_0)}{\sum_{i=1}^{h} \nu_i Z_i/(1+\alpha_i\theta_*)} > C_1 \iff \frac{\sum_{i=1}^{h} \nu_i Z_i\left(\frac{1}{1+\alpha_i\theta_0} - \frac{1}{1+\alpha_i\theta_*}\right)}{\sum_{i=1}^{h} \nu_i Z_i/(1+\alpha_i\theta_*)} > C_1 - 1$$

$$\iff \frac{\sum_{i=1}^{h} \nu_i Z_i \alpha_i/\left((1+\alpha_i\theta_0)(1+\alpha_i\theta_*)\right)}{\sum_{i=1}^{h} \nu_i Z_i/(1+\alpha_i\theta_*)} > (C_1 - 1)/(\theta_* - \theta_0).$$

When $\theta_* \to \theta_0^+$ the limiting statistic is

$$NP(\theta_0, \theta_0, t) = \frac{\sum_{i=1}^{h} \nu_i Z_i \alpha_i/(1+\alpha_i\theta_0)^2}{\sum_{i=1}^{h} \nu_i Z_i/(1+\alpha_i\theta_0)}$$

and the critical value C_{p_1} is obtained from

$$\Pr\left\{\sum_{i=1}^{h} (w_i - C_{p_1})\chi^2_{\nu_i} > 0\right\} = p_1 \qquad \text{for } w_i = \alpha_i/(1+\alpha_i\theta_0).$$

After similar calculations for $\theta_* < \theta_0$, i.e., when $\theta_* \to \theta_0^-$ we find a critical value C_{p_2} of the test $\phi(t)$ from

$$\Pr\left\{\sum_{i=1}^{h}(w_i - C_{p_2})\chi^2_{\nu_i} > 0\right\} = 1 - p_2 \quad \text{for} \quad w_i = \alpha_i/(1+\alpha_i\theta_0)\,.$$

□

Note. A similar way of approach in this problem has been presented by Lin and Harville (1991) and for testing of one-sided hypotheses by Westfall (1989). Having obtained the locally best invariant unbiased test the questions arise: Is our statistical inference now correct? Is it optimal? Maybe a confidence interval not connected with LBIU test will be more useful. Confidence intervals and tests of hypotheses are procedures for making statistical inferences that attach measures of "uncertainty". Several authors have proved in their studies that it is almost always the case that the confidence intervals are "uniformly more informative" than hypothesis tests for making decisions based on parametric values (see Burdick and Graybill 1992, Wonnacott 1987). Therefore, in the next section, as an alternative approach we construct a confidence interval for variance σ_1^2 based on results from optimal point estimation.

6. Alternative confidence interval

It follows from Gnot and Kleffe (1983) that for a given function $f_1\sigma_1^2 + f_2\sigma^2$ the class of admissible invariant quadratic unbiased estimators in the model given by (2) for $k=1$ coincides with the linear combinations of Z_i of the form

$$\hat{\gamma}(u,v) = \sum_{i=1}^{h}(\lambda_1\alpha_i + \lambda_2)\nu_i w_i(u,v) Z_i\,, \quad u,v \geq 0\,,$$

where $w_i(u,v) = \left(1 + 2u\alpha_i + (u^2+v)\alpha_i^2\right)^{-1}$, or

$$\hat{\gamma}(\infty) = \sum_{i=1}^{h-1}\frac{\lambda_1\nu_i}{\alpha_i}Z_i + \lambda_2\nu_h Z_h\,.$$

Here λ_1 and λ_2 are chosen such that $\hat{\gamma}(u,v)$ or $\hat{\gamma}(\infty)$ is unbiased for $f_1\sigma_1^2 + f_2\sigma^2$, i.e.,

$$\begin{cases} \sum_{i=1}^{h}(\lambda_1\alpha_i + \lambda_2)w_i(u,v)\alpha_i\nu_i = f_1\,, \\ \sum_{i=1}^{h}(\lambda_1\alpha_i + \lambda_2)w_i(u,v)\nu_i = f_2 \end{cases}$$

for $\hat{\gamma}(u,v)$, while for $\hat{\gamma}(\infty)$ we have

$$\lambda_1 \operatorname{rank}(W) = f_1 \qquad \text{and} \qquad \lambda_1 \sum_{i=1}^{h-1} \frac{\nu_i}{\alpha_i} + \lambda_2 \nu_h = f_2 \,.$$

The estimator $\hat{\gamma}(u,v)$ is bayesian invariant quadratic unbiased estimator with respect to the prior distribution ρ on (σ_1^2, σ^2) such that $\mathrm{E}_\rho(\sigma_1^2) = u$, $\mathrm{E}_\rho(\sigma^2) = 1$, $\mathrm{Var}_\rho(\sigma_1^2) = v$, $\mathrm{Var}_\rho(\sigma^2) = 0$, while $\hat{\gamma}(\infty)$ is as an unique limit of $\hat{\gamma}(u,v)$ if v tends to infinity.

Now, we present the construction of an exact $1-p$ confidence interval for σ_1^2 based on BIQUE of σ_1^2 according to the following algorithm:

1. Choose the BIQUE $\hat{\sigma}_1^2 = \sum_{i=1}^{h} a_i Z_i$ of σ_1^2 with respect to the prior distribution ρ on (σ_1^2, σ^2):

$$\mathrm{E}(\hat{\sigma}_1^2) = \sigma_1^2 \,; \quad \sum_{i=1}^{h} a_i \alpha_i = 1 \,; \quad \sum_{i=1}^{h} a_i = 0 \,.$$

2. Calculate the variance of $\hat{\sigma}_1^2$

$$\mathrm{Var}(\hat{\sigma}_1^2) = 2\sigma_1^4 \sum_{i=1}^{h} \frac{a_i^2}{\nu_i} (1/\theta + \alpha_i)^2 \,.$$

3. Determine the exact probability distribution of $\hat{\sigma}_1^2$

$$\hat{\sigma}_1^2 \sim \sigma_1^2 \sum_{i=1}^{h} \frac{a_i}{\nu_i} (1/\theta + \alpha_i) \chi^2_{\nu_i} \,,$$

so that for fixed σ_1^2 and for each $\theta \in (0, \infty)$ we have

$$\frac{\hat{\sigma}_1^2}{\sigma_1^2} \sim \sum_{i=1}^{h} \frac{a_i}{\nu_i} (1/\theta + \alpha_i) \chi^2_{\nu_i} = \sum_{i=1}^{h} \mathrm{S}E_\theta(a_i Z_i) \chi^2_{\nu_i} \,,$$

where $\mathrm{SE}(\cdot)$ determines the standard error of an estimator.

4. On the basis of the distribution of quadratic forms find the quantiles C_{p_1} and C_{p_2} such that

$$\Pr\left\{ C_{p_1}(\theta) \le \frac{\hat{\sigma}_1^2}{\sigma_1^2} \le C_{p_2}(\theta) \right\} = 1 - p_1 - p_2 = 1 - p$$

or

$$\Pr\{ \hat{\sigma}_1^2 / C_{p_2}(\theta) \le \sigma_1^2 \le \hat{\sigma}_1^2 / C_{p_1}(\theta) \} = 1 - p_1 - p_2 = 1 - p \,.$$

5. Optimal choice of $\big(C_{p_1}(\theta),\ C_{p_2}(\theta)\big)$

   (a) choose the optimal pair $\big(C^*_{p_1}(\theta),\ C^*_{p_2}(\theta)\big)$ for fixed θ:

$$\big(C^*_{p_1}(\theta), C^*_{p_2}(\theta)\big) = \mathrm{Arg}\Big\{ \min_{\substack{C_{p_1}(\theta), C_{p_2}(\theta) \\ p_1+p_2=p}} \big(1/C_{p_1}(\theta) - 1/C_{p_2}(\theta)\big) \Big\}.$$

   (b) find $\theta^\star$ for $\theta \in (0,\infty)$:

$$\theta^* = \mathrm{Arg}\big\{\max_{\theta}\big(1/C^*_{p_1}(\theta) - 1/C^*_{p_2}(\theta)\big)\big\}.$$

This *maxmin* choice of θ^* protects against a possible worst "scenario".

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