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TESTING HYPOTHESES FOR LINEAR FUNCTIONS OF PARAMETERS IN MIXED LINEAR MODELS

Andrzej Michalski — Roman Zmyślony

ABSTRACT. In the paper an effective method of testing hypotheses for fixed effects and variance components in mixed linear model is presented. The well known F-test for vanishing linear estimable functions of fixed effects and single variance components is derived from quadratic unbiased estimators of corresponding quadratic function of fixed parameters or variance components. The test rejects null hypothesis if the ratio of positive and negative part of this estimator is sufficiently large. This approach gives unified theory of testing hypotheses both for fixed effects and variance components.

1. Introduction

In the paper we deal with the usual mixed linear models. Thus the natural parameter space contains variance components and parameters corresponding to the fixed effects. In this paper we present a relationship between quadratic estimation and testing hypotheses for some linear functions of the parameters in the model. In the problem of testing hypotheses for fixed parameters it is the well known F-test which accepts null hypotheses if the ratio of the quadratic lengths of residuals under hypothesis and model is less than a given critical value. In the paper of Michalski and Zmyślony [4], a test for vanishing a single variance component in mixed linear model is proposed. A null hypotheses is rejected if the ratio of the positive and negative part of the locally best quadratic unbiased estimator of this component is sufficiently large. In this paper it is proved that F-test can be derived in the same way, it means as a ratio of the positive and negative part of a quadratic unbiased estimator for a corresponding quadratic function connected with null hypothesis. Thus we obtained unified theorems for constructing tests for hypotheses about both fixed effects and variance components.

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Throughout the paper, for a given matrix A we use the following notations. The symbols $R(A)$, $N(A)$, A', $r(A)$ stand for range, kernel, transpose and rank of the matrix A, respectively. Moreover, for a symmetric matrix A, nonnegative definite matrices A_+ and A_- stand for positive and negative part of the matrix A, i.e., $A = A_+ - A_-$ and $A_+A_- = 0$. Finally, for a given vector z, the symbol $\operatorname{diag}(z)$ stands for diagonal matrix with the diagonal elements z.

2. The mixed linear model

The model analyzed here is a mixed model given by

$$y = X\beta + \sum_{i=1}^{a} X_i\beta_i + e\,, \tag{2.1}$$

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

$$E(y) = X\beta\,, \qquad \operatorname{Var}(y) = \sum_{i=1}^{a} \sigma_i^2 X_i X_i' + \sigma^2 I_n\,. \tag{2.2}$$

The usual problem for such model is testing hypothesis for linear estimable functions, say $H'\beta$, where H is a $p \times k$ matrix. It is well known that the functions $H'\beta$ are estimable if and only if there exists a $p \times k$ matrix Λ such that

$$H = X'X\Lambda\,. \tag{2.3}$$

Let us consider the following three hypotheses

$$\mathbf{H}_0\colon H'\beta = 0 \quad \text{vs.} \quad \mathbf{H}_1\colon H'\beta \neq 0\,, \tag{2.4}$$

$$\mathbf{H}_0^*\colon \beta' H H'\beta = 0 \quad \text{vs.} \quad \mathbf{H}_1^*\colon \beta' H H'\beta > 0\,, \tag{2.5}$$

and

$$\mathbf{H}_{0,\Lambda}\colon \beta' H(\Lambda' X' X\Lambda)^+ H'\beta = 0 \quad \text{vs.} \quad \mathbf{H}_{1,\Lambda}\colon \beta' H(\Lambda' X' X\Lambda)^+ H'\beta > 0\,. \tag{2.6}$$

Here C^+ stands for Moore-Penrose general inverse of C. Now we prove the following

Lemma 2.1. *The hypotheses* (2.4), (2.5) *and* (2.6) *are equivalent.*

P r o o f. The equivalence of (2.4), (2.5) is obvious. To prove that (2.5) and (2.6) are equivalent note that in view of (2.3) hypotheses $\mathbf{H}_0^*$ and $\mathbf{H}_{0,\Lambda}$ can be written as $\beta' X' X \Lambda\Lambda' X' X\beta = 0$ and $\beta' X' X\Lambda(\Lambda' X' X\Lambda)^+ \Lambda' X' X\beta = 0$, respectively. Since $X\Lambda(\Lambda' X' X\Lambda)^+\Lambda' X'$ is an orthogonal projector on $R(X\Lambda\Lambda' X')$ we have

$$R(X\Lambda\Lambda' X') = R\big(X\Lambda(\Lambda' X' X\Lambda)^+\Lambda' X'\big)$$

and thus the lemma follows. □

3. Test for estimable functions for Gauss-Markov model

Throughout this section we deal with Gauss-Markov model, i.e.,

$$E(y) = X\beta\,, \qquad \mathrm{Var}(y) = \sigma^2 I_n\,. \tag{3.1}$$

For this model we present the construction of test for hypothesis (2.4), where the matrix H satisfies (2.3), i.e., estimability condition. It is well known that for hypothesis (2.4) there exists F-test if

$$r = r(X) < n\,. \tag{3.2}$$

For testing $\mathbf{H}_0^*$ or $\mathbf{H}_{0,\Lambda}$ we need a quadratic unbiased estimator for a quadratic function of β. Thus we give the following

Definition 3.1. We say that the function $\beta' C\beta$ is quadratic estimable if there exists a matrix A such that $Ey'Ay = \beta' C\beta$.

In the following lemma we prove that conditions (2.3) and (3.2) imply that there exists the best quadratic unbiased estimator (BQUE for short) of $\beta' HH'\beta$.

Lemma 3.1. *If $H'\beta$ are estimable and if* (3.2) *holds, then the function $\beta' HH'\beta$ is quadratic estimable. Moreover, $y'Ay$ is* BQUE *of $\beta' HH'\beta$ with $A_+ = X\Lambda\Lambda' X'$ and $A_- = \mathrm{tr}(H\Lambda')M$, where $M = I_n - XX^+$.*

P r o o f. If $H'\beta$ is estimable, then according to (2.3) we have $H = X' X\Lambda$. Note that $H'\widehat{\beta}$ is the best linear unbiased estimator for $H'\beta$, where

$$\widehat{\beta} = (X' X)^+ X' y\,. \tag{3.3}$$

Moreover, because of (3.2), there exists BQUE of σ^2, i.e.,

$$\widehat{\sigma^2} = y' My/(n-r)\,. \tag{3.4}$$

From (2.3) and (3.3) it follows that

$$E\big(\widehat{\beta}' HH'\widehat{\beta}\,\big) = E\big(\widehat{\beta}' X' X\Lambda\Lambda' X' X\widehat{\beta}\,\big) = E(y' X\Lambda\Lambda' X' y)\,.$$

Making several times the use of $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ and $E(yy') = X\beta\beta'X' + \sigma^2 I_n$ we get

$$\begin{aligned} E(y'X\Lambda\Lambda'X'y) &= E\big(\operatorname{tr}(X\Lambda\Lambda'X'yy')\big) \\ &= \operatorname{tr}\big(X\Lambda\Lambda'X'(X\beta\beta'X' + \sigma^2 I_n)\big) \\ &= \beta'HH'\beta + \sigma^2 \operatorname{tr}(H\Lambda'). \end{aligned}$$

From the above and (3.4) it follows that $\widehat{\beta}'HH'\widehat{\beta} - \operatorname{tr}(H\Lambda')\widehat{\sigma}^2$ is BQUE of $\beta'HH'\beta$ and $A_+ = X\Lambda\Lambda'X'$, $A_- = \operatorname{tr}(H\Lambda')/(n-r)M$. Since $R(A_+) \subset R(X)$ and $R(M) = N(X')$, we have $A_+A_- = 0$. □

Remark 3.1. In fact, the estimator $\widehat{\beta}'HH'\widehat{\beta} - \operatorname{tr}(H\Lambda')\widehat{\sigma}^2$ of $\beta'HH'\beta$ is the best unbiased estimator, because it is a function of the complete sufficient statistics (see Lehman [3], Rao [5], or Zmyślony [7].

Now, in order to construct a test for hypotheses (2.5) or (2.6) we can adopt the approach introduced by Michalski and Zmyślony [4]. According to Lemma 2.1 those hypotheses are equivalent, however, it is useful to consider (2.6).

THEOREM 3.2. *Under hypothesis* $\mathbf{H}_{0,\Lambda} : \beta'H(\Lambda'X'X\Lambda)^+H'\beta = 0$, *the ratio*

$$F = \frac{\widehat{\beta}'X'X\Lambda(\Lambda'X'X\Lambda)^+\Lambda'X'X\widehat{\beta}}{\operatorname{rank}(H)\widehat{\sigma}^2} \tag{3.5}$$

or, equivalently,

$$F = \frac{y'X\Lambda(\Lambda'X'X\Lambda)^+\Lambda'X'y}{\operatorname{rank}(H)\widehat{\sigma}^2} \tag{3.6}$$

is F-distributed with $\nu_1 = \operatorname{rank}(H)$ *degrees of freedom for nominator and* $\nu_2 = n - \operatorname{rank}(X)$ *degrees of freedom for denominator.*

Proof. First note that equivalence of (3.5) and (3.6) follows from (3.3). Let $H_* = HD^{1/2}$ and let $\Lambda_* = \Lambda D^{1/2}$, where $D = (\Lambda'X'X\Lambda)^+$. From Lemma 3.1 it follows that the corresponding $A_+^* = X\Lambda(\Lambda'X'X\Lambda)^+\Lambda'X'$ and $A_-^* = \operatorname{tr}(H_*\Lambda_*')/(n-r)M$. Note that A_+^* and M are idempotent matrices. Moreover,

$$\begin{aligned} \operatorname{tr}\big(H_*\Lambda_*'\big) &= \operatorname{tr}\big(X'X\Lambda(\Lambda'X'X\Lambda)^+\Lambda'\big) \\ &= \operatorname{tr}\big(X\Lambda(\Lambda'X'X\Lambda)^+\Lambda'X'\big) \\ &= \operatorname{rank}\big(X\Lambda(\Lambda'X'X\Lambda)^+\Lambda'X'\big) \\ &= \operatorname{rank}(H). \end{aligned}$$

Thus $y'A_+^*y/\sigma^2 = \widehat{\beta}'X'X\Lambda(\Lambda'X'X\Lambda)^+\Lambda'X'X\widehat{\beta}/\sigma^2$ under $\mathbf{H}_{0,\Lambda}$ is chi-square distributed with $\operatorname{rank}(H)$ degrees of freedom. Now, because of $y'My/\sigma^2 =$

$(n-r)\widehat{\sigma}^2/\sigma^2$ is chi-square distributed with n- rank(X) degrees of freedom, the theorem follows. □

Remark 3.2. Note that $F = y'A^*_+y/y'A^*_-y$ and $E(y'A^*_+y) = E(y'A^*_-y)$ under $\mathbf{H}_{0,\Lambda}$, while $E(y'A^*_+y) > E(y'A^*_-y)$ under $\mathbf{H}_{1,\Lambda}$. Therefore it is reasonable to reject null hypothesis if F is greater than the critical value $F_\alpha(v_1, v_2)$ at significance level α. One can prove that this test is equivalent to the analysis of variance F-test.

4. Test for estimable functions in general linear model

In this section we extend the construction of test for hypothesis (2.6) on the general linear model given by (2.1), it means that the vector of observations

$$y \sim N_n\Big(X\beta\,,\ \sum_{i=1}^{a}\sigma_i^2 V_i + \sigma^2 I_n\Big),$$

where $V_i = X_i X_i'$ for $i = 1, \ldots, a$.

As in previous section, we consider the problem of testing hypothesis

$$\mathbf{H}_{0,\Lambda} : \beta' H(\Lambda' X' X \Lambda)^+ H'\beta = 0$$

or, equivalently,

$$\mathbf{H}_{0,\Lambda} : \beta' H_* H_*'\beta = 0\,,$$

where $H_* = HD^{1/2}$ and $\Lambda_* = \Lambda D^{1/2}$, while $D = (\Lambda' X' X\Lambda)^+$. Define $M_* = I_n - X_* X_*^+$ with $X_* = X'X + \sum_{i=1}^{a} V_i$.

Theorem 4.1. *Suppose that the following conditions are satisfied*

(A1) rank$(X_*) = l < n$,

(A2) $\Lambda X' V_i = 0$ *for* $i = 1, \ldots, a$.

Then $\widehat{\beta}' H_* H_*'\widehat{\beta} - h\widehat{\sigma}^2$, *where* $h = \operatorname{rank}(H)$, *is a quadratic unbiased estimator of* $\beta' H_* H_*'\beta$ *and* $l\widehat{\sigma}^2/\sigma^2$ *is centrally chi-square distributed with* $n-l$ *degrees of freedom, while under* $\mathbf{H}_{0,\Lambda}$ *the random variable* $\widehat{\beta}' H_* H_*'\widehat{\beta}/\sigma^2$ *has central chi-square distribution with* h *degrees of freedom.*

P r o o f. On can easily check that condition (A1) guaranties existence of an unbiased estimator of σ^2, namely $\widehat{\sigma}^2 = y' M_* y/(n-l)$. Following proof of Theorem 3.2 and using conditions (A1) and (A2) we get the proof of the theorem. □

5. Examples

EXAMPLE 5.1. One-way analysis of variance model.

Let us consider the fixed model corresponding to the one way classification, i.e.,

$$y_{ij} = \beta_i + e_{ij}\,, \quad i = 1, \dots, k\,, \quad j = 1, \dots, n_i\,, \tag{5.1}$$

$$n = \sum_{i=1}^{k} n_i \text{ is a total number of observations}. \tag{5.2}$$

The usually tested hypothesis is $\beta_1 = \cdots = \beta_k$, which can be written in the matrix form as $\mathbf{H}_0$: $H'\beta = 0$ with a matrix

$$H = \begin{pmatrix} 1'_{k-1} \\ -\mathbf{I}_{k-1} \end{pmatrix},$$

where $1'_{k-1}$ is $k-1$-vector of one's, while $\mathbf{I}_{k-1}$ is the identity matrix. If the vector of observations is in the lexicographical order, then

$$\Lambda = (X'X)^{-1}H = \begin{pmatrix} \frac{1}{n_1} 1'_{k-1} \\ -R^{-1}_{k-1} \end{pmatrix},$$

where R_{k-1} is the $(k-1) \times (k-1)$ diagonal matrix with n_i on the diagonal except n_1, i.e., $R_{k-1} = \operatorname{diag}(n_2, \dots, n_k)$. Now, after simple calculations we find that

$$\Lambda(\Lambda'X'X\Lambda)^{-1}\Lambda' = R^{-1} - \frac{1}{n} 1_k 1'_k\,,$$

where $R = \operatorname{diag}(r_k)$, while $r_k = (n_1, \dots, n_k)$. Note that $y'X = (y_{1.}, \dots, y_{k.})$, where $y_{i.} = \sum_{j=1}^{n_i} y_{ij}$. Now, using the usual notation $y_{...}$ for total yield of observations, according to Theorem 3.2, we get the numerator of F test as

$$y'X\left(R - \frac{1}{n} 1_k 1'_k\right)X'y = \sum_{i=1}^{k} \frac{y_{i.}^2}{n_i} - \frac{y_{...}^2}{n}\,, \tag{5.3}$$

which is a well known sum of squares for the model in one-way analysis of variance.

EXAMPLE 5.2. Block design model.

Consider an experiment with v treatments arranged in b blocks according to the $v \times b$ incidence matrix N with the total number of observations n. Let $y = (y_1, \dots, y_n)'$ be an $n \times 1$ vector of observations and follow the model

$$y = (\Delta', D')(\gamma', \beta')' + e\,, \tag{5.4}$$

where Δ' is the $n \times v$ matrix with elements δ_{il} being 0 or 1, according as y_i receives the l treatment or not; D' is the $n \times b$ matrix with elements d_{ij} being 1 or 0 according as y_i is in jth block or not. As usual, γ and β are the $v \times 1$ vector of treatments effects and $b \times 1$ vector of block effects, respectively. Note that the incidence matrix $N = \Delta D'$. As usual, let $r = (r_1, \dots, r_v)' = N1_b$ and $k = (k_1, \dots, k_b)' = N'1_v$ stand for vectors of treatment replications r_i and block sizes k_j, respectively. Here 1_c stands for $c \times 1$ vector with all elements 1. Further, let $R = \operatorname{diag}(r)$, and $K = \operatorname{diag}(k)$. Note that $\Delta\Delta' = R$ and $DD' = K$. We shall deal with one of two cases, which have been considered by Kageyama and Zmyślony [2], namely:

(a) γ is a vector of fixed parameters and β is a random vector normally distributed $N(0, \sigma_1^2 I)$.

(b) β is a vector of fixed parameters and γ is a random vector normally distributed $N(0, \sigma_1^2 I)$.

From the above mentioned paper it follows that in the case (a) there exists the best unbiased estimator for each linear estimable function if and only if the incidence matrix is of the form $N = \frac{1}{b} r 1_b'$ provided a block design is β-connected, i.e., $r(K - N'R^{-1}N) = b - 1$. In this case to test hypothesis $\mathbf{H}_0 :$ $\gamma_1 = \dots = \gamma_v$ we have $X'X = \Delta\Delta'$ and $(X'X)^{-1} = R^{-1}$. Next $V_1 = DD'$ implies that

$$\Lambda' X V_1 = H'(X'X)^{-1}\Delta' DD' = H' R^{-1} N D' = H' 1_v r' = 0$$

because the rows of H' are contrasts. Thus in view of Theorem 4.1 we conclude that F statistics, for all treatment contrasts to be equal zero, is distributed $F_{v-1, n-v-b+1}$. It is clear that the numerator of F is given by (5.3) with $y_{i.} = y_{T_i}$ and $n_i = r_i$, where y_{T_i} is the total yield over the ith treatment, while estimator $\widehat{\sigma}^2$ for σ^2 is given in the paper Kageyama, Zmyślony [2] (see Theorem 4.1) and is given by

$$\widehat{\sigma}^2 = \frac{1}{n - v - b + 1}[SSE - SSB],$$

where

$$SSE = \sum_{i=1}^{n} y_i^2 - \sum_{j=1}^{v} \frac{y_{T_j}^2}{r_i},$$

while

$$SSB = \sum_{j=1}^{v} \frac{y_{B_j}^2}{k} - \frac{y_.^2}{n}.$$

Here k is a common block size, while y_{B_j} is the total yield of observation over the jth block and $y_.$ is a total yield of observation.

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Andrzej Michalski
Agriculture University of Wrocław
PL–50–357 Wrocław
ul. Grunwaldzka 53
POLAND
E-mail: max@ozi.ar.wroc.pl.

Roman Zmyślony
Institute of Mathematics
Technical University
PL–Zielona Góra
ul. Podgórna 50
POLAND
E-mail: R.Zmyslony@im.pz.zgora.pl