CONFIDENCE REGIONS FOR VARIANCE COMPONENTS
IN UNBALANCED MIXED LINEAR MODELS

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ABSTRACT

We present a general procedure for obtaining exact confidence
regions for the variance components in unbalanced mixed linear models.
The procedure utilizes, as pivotal quantities, quadratic forms that may
depend on the variance components in a complicated way and that are dis-
tributed independently as chi-square variates. In the special case of
balanced classificatory models, the pivotal quantities simplify to scalar
multiples of sums of squares from the usual analysis of variance. The
procedure can be easily modified so as to obtain an exact confidence
region for ratios of variance components and can be regarded as a
generalization of Wald's procedure for obtaining a confidence interval
for a single variance ratio.
1. INTRODUCTION

Suppose that \( y \) is an \( n \times 1 \) observable vector that follows the general mixed linear model

\[
y = X_0 \beta_0 + X_1 b_1 + \ldots + X_k b_k + b_{k+1}
\]

where \( X_i \) is an \( n \times m_i \) known matrix \( (i = 0, \ldots, k) \), and \( \beta_0 \) is an \( m_0 \times 1 \) vector of unknown parameters, \( b_i \) is an \( m_i \times 1 \) unobservable random vector whose distribution is \( N(0, \sigma_i^2 I) \), that is, multivariate normal with mean vector 0 and variance-covariance matrix \( \sigma_i^2 I \) \((i=1,\ldots,k+1)\), and \( \sigma_1^2, \ldots, \sigma_k^2 \) are unknown parameters. Assume that \( b_1, \ldots, b_{k+1} \) are independently and that \( \sigma_i^2 > 0 \) \((i=1,\ldots,k)\) and \( \sigma_{k+1}^2 > 0 \). Define

\[
\sigma^2 = (\sigma_1^2, \ldots, \sigma_k^2, \sigma_{k+1}^2)^T, \quad \gamma_i = \frac{\sigma_i^2}{\sigma_{k+1}^2} \quad (i = 1, \ldots, k) \text{ and } \\
\gamma = (\gamma_1, \ldots, \gamma_k)^T.
\]

We devise an exact 100 \((1-\alpha)\)% confidence region for the vector \( \sigma^2 \) of variance components. Essentially the same approach can be used to obtain an exact 100 \((1-\alpha)\)% confidence region for the vector \( \gamma \) of variance ratios. Confidence regions for \( \sigma^2 \) and \( \gamma \) can be of direct interest. They can also be used to obtain (generally conservative) confidence intervals for functions of \( \sigma^2 \) or \( \gamma \) (Spjotvoll, 1972; Khuri, 1981) and for linear combinations of the fixed and random effects, that is, linear combinations of the elements of the vectors \( \beta_0, b_1, \ldots, b_k \) (Jeske, 1985).

Let \( \chi^2(f) \) represent a chi-square distribution with \( f \) degrees of freedom, and take \( \chi_{\alpha,f}^2 \) to be the upper-\( \alpha \) point of this distribution. Under certain circumstances, there exist \( k+1 \) quadratic forms
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\[ y^T A_1 y, \ldots, y^T A_{k+1} y, \] where \( A_1, \ldots, A_{k+1} \) are \( n \times n \) symmetric matrices of known constants, such that (i) \( y^T A_1 y, \ldots, y^T A_{k+1} y \) are distributed independently, (ii) \( y^T A_i y/(\sigma^2_{k+1} c_i) \sim \chi^2(f_i) \) for a positive integer \( f_i \) and a scalar \( c_i \) that are necessarily given by \( f_i = \text{rank}(A_i) \) and \( c_i = f_i^{-1}(d_{i,k+1} + \sum_{j=1}^{k+1} d_{ij} y_j) \) with \( d_{ij} = \text{tr}(X_j^T A_i X_j) \) (\( j=1, \ldots, k \)) and \( d_{i,k+1} = \text{tr}(A_i) \) (\( i=1, \ldots, k+1 \)), and (iii) the \( (k+1) \times (k+1) \) matrix with \( ij^{th} \) element \( d_{ij} \) is nonsingular. If the \( k+1 \) quadratic forms \( y^T A_1 y, \ldots, y^T A_{k+1} y \) exist, then clearly, for \( 0 < \alpha < 1 \), a \((1-\alpha)\%)\ confidence region for the vector \( \sigma^2 \) is given by the set \( S(y) \) consisting of those values of the vector \( \sigma^2 \) that simultaneously satisfy the \( k+1 \) inequalities

\[ x_{1-\alpha_{12},f_i}^* \leq y^T A_i y/(\sigma^2_{k+1} c_i) \leq x_{\alpha_{11},f_i}^* \quad (i=1, \ldots, k+1), \]

where \( \alpha_{11} \) and \( \alpha_{12} \) represent nonnegative constants such that
\[ \alpha_{11} + \alpha_{12} < 1 \quad (i=1, \ldots, k+1) \quad \text{and} \quad \Pi_{i}(1-\alpha_{11} - \alpha_{12}) = 1-\alpha. \]

It is well known that, for balanced classificatory models, the requisite quadratic forms exist and, in fact, can be taken to be those sums of squares in the customary analysis of variance that correspond to the random effects and errors, in which case \( f_1 + \ldots + f_k = n - \text{rank}(X_0) \) (e.g., Broemeling, 1969). Other special cases for which such quadratic forms have been found are treated by, for example, Broemeling and Bee (1976).
Unfortunately, in many cases, quadratic forms \( y^T A_1 y, \ldots, y^T A_{k+1} y \), whose matrices \( A_1, \ldots, A_{k+1} \) are matrices of known constants and that satisfy the three desired conditions, may, if they exist at all, be hard to find and/or may be such that \( \sum f_i < n - \text{rank}(X_0) \), in which case the confidence region \( S(y) \) may be overly large. In what follows, we present a general procedure for forming an exact 100(1-\(\alpha\))% confidence region for the vector \( \sigma^2 \). Our approach differs from the aforementioned approach in that we allow the elements of the matrix \( A_i \) of the \( i \)th quadratic form \( y^T A_i y \) to be functionally dependent on the last \( k-i+1 \) variance ratios \( \gamma_i = \frac{\sigma_i^2}{\sigma_{k+1}^2}, \ldots, \gamma_k = \frac{\sigma_k^2}{\sigma_{k+1}^2} \) (\( i=1, \ldots, k \)). By allowing this dependence, we are able to construct quadratic forms \( y^T A_1 y, \ldots, y^T A_{k+1} y \) that satisfy the three desired properties and which, in addition, are such that \( \sum f_i = n - \text{rank}(X_0) \). Then, as in the aforementioned approach, an exact 100(1-\(\alpha\))% confidence region consists of the set \( S(y) \) of all values of the vector \( \sigma^2 \) that simultaneously satisfy the \( k+1 \) inequalities (1.2).

Our procedure can be regarded as an extension of Wald's (1940 and 1947) procedure. Wald's procedure, when extended along the lines discussed by Thompson (1955), Spjotvoll (1968), Seely and El-Bassiouni (1983), and Harville and Fenech (1984), covers the special case \( k=1 \). Hartley and Rao (1967, Sec. 9) proposed a general procedure for obtaining an exact 100 (1-\(\alpha\))% confidence region which, like ours, can be viewed as a generalization of Wald's procedure. However, as can easily be shown, it produces confidence regions of a seemingly unappealing form and, in fact, can with high probability produce confidence regions of infinite volume.
In principle, the likelihood ratio could be used to generate a confidence region (Hartley and Rao, 1967, Sec. 8). However, the percentiles of its distribution are approximated on the basis of asymptotic results. The accuracy of these approximations is questionable and is not easily investigated. (What few asymptotic results are available for mixed linear models—see, for example, Miller (1977)—seem unassuring, and, except in special cases, Monte Carlo studies are computationally unfeasible.)

2. PRELIMINARIES

Define $V_1 = I + \sum_{s=1}^{k+1} \gamma s X s T$ ($i=0,...,k-1$) and $V_{k+1} = V_k = I$, and let $V = V_0 = I + \sum_{s=1}^{k} \gamma s X s T$. Under the assumed model (1.1), $y \sim N(\beta_0, \sigma^2_{k+1} V)$, and the parameter space for the vector $\sigma^2$ is

$\Omega_0 = \{\sigma^2 : \sigma^2_{k+1} > 0, \gamma_i > 0 (i=1,...,k)\}.$

Note, however, that the matrix $V$ is positive definite for some values of the vector $\gamma$ that include one or more negative elements.

Subsequently, we take the model to be the generalization of model (1.1) that results from disregarding our original definitions of $\sigma^2_1,...,\sigma^2_{k+1}$ as variances and from assuming only that $y \sim N(\beta_0, \sigma^2_{k+1} V)$ and that the parameter space for the vector $\sigma^2$ is

$\Omega = \{\sigma^2 : \sigma^2_{k+1} > 0, (\gamma_{i+1},...,\gamma_k)^T \in \Gamma_i (i=0,...,k-1)\},$
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where \( r \) is the set of all values of \((y_{i+1}, \ldots, y_k)^T\) such that \( V_i \) is positive definite.

We shall have occasion to refer to a model, to be called Model \( i \), in which

\[
y = X_0 \beta_0 + X_1 \beta_1 + \ldots + X_i \beta_i + e_i,
\]

where \( \beta_1, \ldots, \beta_i \) are vectors which, like \( \beta_0 \), are composed of unknown parameters, where \( e_i \) is an \( n \times 1 \) unobservable random vector with \( \text{E}(e_i) = 0 \) and \( \text{var}(e_i) = \sigma_i^2 X_i V_i \), and where \( y_{i+1}, \ldots, y_k \) and hence \( V_i \) are assumed to be known \((i=1, \ldots, k)\). Model \( i \) is essentially the same as model (1.1) except that the parameter vectors \( \beta_1, \ldots, \beta_i \) appear in place of the random vectors \( b_1, \ldots, b_i \) and the parameters \( y_{i+1}, \ldots, y_k \) are taken to be known instead of unknown.

For \( i = 0, 1, \ldots, k \), define \( X_i^* = (X_0, X_1, \ldots, X_i) \). Note that \( X_i^* = (X_{i-1}, X_i) \) \((i=1, \ldots, k)\). Let \( r_0 = \text{rank}(X_0) \), \( r_i = \text{rank}(X_i^*) - \text{rank}(X_{i-1}^*) \) \((i=1, \ldots, k)\), and \( r_{k+1} = n - \text{rank}(X_k^*) \). Subsequently, we assume that \( r_i > 0 \) \((i=1, \ldots, k+1)\).

We write \( A^- \) for an arbitrary generalized inverse of a matrix \( A \), that is, \( A^- \) is any matrix satisfying \( AA^-A = A \). Define

\[
P_{i-1} = X_{i-1} (X_{i-1}^T V_i^{-1} X_{i-1})^{-1} X_{i-1}^T V_i^{-1} \quad (i=1, \ldots, k+1).
\]

Note that

\[
P_i^2 = P_{i-1}, \quad P_i^T V_i^{-1} = (V_i^{-1} P_{i-1})^T = V_i^{-1} P_{i-1}
\]

and that \( P_{i-1} X_{i-1}^* = X_{i-1}^* \) and \( X_{i-1}^* V_i^{-1} P_{i-1} = (P_{i-1} X_{i-1}^*)^T V_i^{-1} = X_{i-1}^* V_i^{-1} \),
implying that, for $j = 0, \ldots, i-1$,

$$P_{i-1}X_j = X_j, X_j' P_{i-1} = X_j' P_{i-1}^*- X_j' V_{i-1}^* P_{i-1} = X_j' V_{i-1}^*$$

(i=1, ..., k+1). Note also that, since the matrix $I-P_k = I - X_k' X_k$ is symmetric and idempotent, there exists an $n \times r_{k+1}$ matrix $F$ such that $I-P_k = FF^T$ and $F^TF = I$ and that $F^T X_k = 0$, implying that $F^T X_i = 0$ (i=0, ..., k).

3. QUADRATIC FORMS

3.1 Definition

We now introduce the quadratic forms on which the proposed confidence region is to be based.

Define $C_i = X_i' V_{i-1} (I-P_{i-1}) X_i$ and $q_i = X_i' V_{i-1} (I-P_{i-1}) y$ (i=1, ..., k).

It is known that rank ($C_i$) = $r_i$ and that there exists an $m_i \times r_i$ matrix $L_i$ of rank $r_i$ such that, under Model i, $\tau_i = L_i^T \delta_i$ would be an estimable parametric function. It is further known that $L_i^T = L_i^T C_i$ for some matrix $L_i$, which is necessarily of rank $r_i$, and that, under Model i, the minimum-variance linear unbiased estimator of $\tau_i$ would be

$$\tilde{\tau}_i = (\tilde{\tau}_{i1}, \ldots, \tilde{\tau}_{ir_i})^T = L_i^T q_i.$$ 

The proposed confidence region is based on the $k+1$ quadratic forms

$$Q_i = Q_i(y_1, \ldots, y_k; y) = \tilde{\tau}_i^T [L_i^T (C_i + \gamma_i^2) L_i]^{-1} \tilde{\tau}_i (i=1, \ldots, k),$$

$$Q_{k+1} = Q_{k+1}(y) = y^T (I-P_k) y = z^T z.$$
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where \( z = F^T y \). As shown in Section 3.2, \( Q_1/\sigma_{k+1}^2, \ldots, Q_{k+1}/\sigma_{k+1}^2 \) are distributed independently as chi-square random variables with degrees of freedom \( r_1, \ldots, r_{k+1} \), respectively. The quadratic forms \( Q_1, \ldots, Q_{k+1} \) are invariant to the choice of the matrices \( A_1, \ldots, A_k \), as is easily verified.

3.2 Joint distribution

Under the assumed distribution for \( y \), which is \( N(\mu_0, \sigma^2 I) \), we find that, for \( j < i = 1, \ldots, k \),

\[
\text{cov}(q_i, q_j) = \sigma^2 \alpha_{k+1} X_i^T V_1^{-1} (I-P_1-I) V_j^{-1} (I-P_j-I) X_j
\]

\[
= \sigma^2 \alpha_{k+1} X_i^T V_1^{-1} (I-P_1-I) (V_1 + \sum_{s=j}^{k} V_s V_s^T) V_j^{-1} (I-P_j-I) X_j
\]

\[
= \sigma^2 \alpha_{k+1} X_i^T V_1^{-1} (I-P_1-I) V_j^{-1} V_j^T (I-P_j-I) X_j
\]

\[
= \sigma^2 \alpha_{k+1} X_i^T V_1^{-1} (I-P_1-I) V_j^{-1} V_j^T (I-P_j-I) X_j
\]

\[
(3.1)
\]

It can be shown, in similar fashion, that \( \text{cov}(z, q_j) = 0 \) (\( j=1, \ldots, k \)).

Thus, \( q_1, \ldots, q_k, z \) are distributed independently, implying that \( \tilde{\tau}_1, \ldots, \tilde{\tau}_k, z \) are distributed independently and hence that \( Q_1, \ldots, Q_k, Q_{k+1} \) are distributed independently.
Further, for $i = 1, \ldots, k$, we find that

\begin{equation}
E(q_i) = X_i^T V_1^{-1} (I - P_{i-1}) X_0 \beta_0 = 0,
\end{equation}

\begin{equation}
\text{var}(q_i) = \sigma^2 \left( X_i^T V_1^{-1} (I - P_{i-1}) V_1 V_1^{-1} (I - P_{i-1}) X_i \right),
\end{equation}

\begin{equation}
= \sigma^2 \left( X_i^T V_1^{-1} (I - P_{i-1}) (V_1 + \gamma_i X_i Y_i^T V_1 V_1^{-1} (I - P_{i-1}) X_i \right),
\end{equation}

implying that $\tau_i \sim N(0, \sigma^2 \left(C_i + \gamma_i C_i^2\right))$, and hence that

\begin{equation}
Q_i / \sigma^2 \sim \chi^2(r_i). \quad \text{Also, } z \sim N(0, \sigma^2 \xi), \quad \text{and, consequently,}
Q_k / \sigma^2 \sim \chi^2(r_{k+1}).
\end{equation}

### 3.3 Canonical representation

We now consider a particular choice for the parameter vectors

$\tau_1, \ldots, \tau_k$ or, equivalently, for the coefficient matrices $A_1^T, \ldots, A_k^T$.

This choice produces representations for the quadratic forms $Q_1, \ldots, Q_k$ that are, as we discuss in Section 4, informative about the nature of the proposed confidence region, and that can be useful computationally.

Let $\Delta_{11}, \ldots, \Delta_{1r_i}$ represent the nonzero, and hence positive, characteristic values of the matrix $C_i$, define $D_i = \text{diag}(\Delta_{11}, \ldots, \Delta_{1r_i})$, and take $R_i$ to be an $m_i \times r_i$ matrix whose columns are orthonormal characteristic vectors of $C_i$ corresponding to the values $\Delta_{11}, \ldots, \Delta_{1r_i}$.
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respectively. Thus, by definition,

\[ C_1 R_1 = R_1 D_1, \quad R_1^T R_1 = I, \]

implying that

\[ R_1^T C_1 R_1 = D_1, \quad R_1^T C_1^2 R_1 = (C_1 R_1)^T C_1 R_1 = D_1 R_1^T R_1 D_1 = D_1^2. \]

Consider the choice

\[ A_1 = D_1^{-1/2} R_1 C_1 \quad \text{to} \quad L_1 C_1 \]

with \( L_1 = D_1^{-1/2} R_1 \). Note that this choice varies with \( y_{i+1}, \ldots, y_k \). It leads to the representation

\[ Q_1 = \tilde{\tau}_1^T (I + y_1 D_1)^{-1} \tilde{\tau}_1 = \sum_{j=1}^{r_1} \frac{\tilde{\tau}_1^2}{1 + y_1 A_{1j}} \]

with \( \tilde{\tau}_1 = D_1^{-1/2} R_1 q_1 \).

3.4 An alternative approach

The quadratic forms \( Q_1, \ldots, Q_{k+1} \) can be defined, and their properties established, via a vector-space approach, as we now demonstrate. Denote by \( R^N \) the vector space consisting of all \( n \)-dimensional real vectors, and let \( W^1 \) represent the orthogonal complement of a subspace \( W \) of \( R^N \) with respect to the usual inner product, that is, the inner product that assigns the value \( y_1^T y_2 \) to any two \( n \)-dimensional real vectors \( y_1 \) and \( y_2 \). Further, let \( W^1 \) represent the orthogonal complement of \( W \) with respect to the inner product \( y_1^T y_2 \). Denote by \( C(A) \) the column space of a matrix \( A \).
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Define $U_{k+1} = (X_k^*)^\perp$ and

$$U_i = (X_{i-1}^*)^\perp \cap [(X_i^*)^\perp] \quad (i=1, \ldots, k).$$

Then, $\dim(U_{k+1}) = r_{k+1}$ and

$$\dim(U_i) = \dim[(X_{i-1}^*)^\perp] - \dim[(X_i^*)^\perp]$$

$$= n - \text{rank}(X_{i-1}^*) - [n - \text{rank}(X_i^*)] = r_i \quad (i=1, \ldots, k).$$

Take $H_i$ to be an $n \times r_i$ matrix whose columns form a basis for $U_i$ $(i=1, \ldots, k+1)$. Derivations paralleling those of results (3.1), (3.2), and (3.3) reveal that $H_i^T V H_j = 0$ $(j<i=1, \ldots, k+1)$, that $H_i^T X_0 = 0$ $(i=1, \ldots, k+1)$, and that $H_i^T V H_i = H_i^T (V_1 + \gamma_i X_1 X_1^T) H_i$ $(i=1, \ldots, k)$ and $H_i^T V H_{k+1} = H_i^T H_{k+1}$. Note that $U_1, \ldots, U_{k+1}$ are orthogonal with respect to the inner product $y_1^T y_2$ and that their direct sum is $C(X_0)^\perp$.

We have, in effect, established that the vectors $H_1 y, \ldots, H_{k+1} y$ are distributed independently, with $H_i^T y \sim N[0, \sigma^2 \gamma_i H_i^T (V_1 + \gamma_i X_1 X_1^T) H_i]$ $(i=1, \ldots, k)$ and $H_{k+1}^T y \sim N(0, \sigma^2 H_{k+1} H_{k+1}^T)$. It follows that the $k+1$ quadratic forms

$$Q_i = y^T H_i (H_i^T (V_1 + \gamma_i X_1 X_1^T) H_i)^{-1} H_i^T y \quad (i=1, \ldots, k)$$

$$Q_{k+1} = y^T H_{k+1} (H_{k+1}^T H_{k+1})^{-1} H_{k+1}^T y$$

are distributed independently, with $Q_i/\sigma^2 \sim \chi^2(r_i)$ $(i=1, \ldots, k+1)$. These quadratic forms are invariant to the choice of the basis matrices $H_1, \ldots, H_{k+1}$, as is easily verified.
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It is easy to show that one choice for the matrices $H_1^T, \ldots, H_k^T$ is

$H_i^T = L_i^T V_i^{-1} (I - P_{i-1}) (i = 1, \ldots, k)$,

$H_{k+1}^T = F^T$. This result can, in turn, be used to show that the quadratic forms $Q_1^*, \ldots, Q_k^*$ are identical to the quadratic forms $Q_1, \ldots, Q_{k+1}$, introduced in Section 3.1. The representations $Q_1, \ldots, Q_{k+1}$ are informative about the nature of the computations required to evaluate the $k+1$ quadratic forms for specified values of $\gamma_1, \ldots, \gamma_k$.

4. NATURE OF CONFIDENCE REGION

4.1 General case

The set $S(y)$, consisting of those values of the vector $\sigma^2 (\sigma^2 \in \Omega)$ that simultaneously satisfy the $k+1$ inequalities

$$
\chi_{i-1, \sigma_{i-1}^2, r_1}^* < Q_i / \sigma_{k+1}^2 < \chi_{i+1, \sigma_{i+1}^2, r_1}^* (i = 1, \ldots, k+1),
$$

is a $100(1-\alpha)$% confidence region for $\sigma^2$. We now present an alternative description of this set, one which provides more insight into the nature of the set and which is more useful computationally.

Let $\lambda_1^*$ represent the maximum characteristic value of the matrix $X_1^T V_1^{-1} X_1$, and define $\Delta_i^* = \max(\Delta_{i1}, \ldots, \Delta_{ir_i}) (i = 1, \ldots, k)$. It is easy to show that $\Delta_i^* < \lambda_i^*$. For any fixed value of $(\gamma_{i+1}, \ldots, \gamma_k) \in \Gamma_i$, the matrix

$V_{i-1} = V_i + \gamma_i X_i^T X_i^T$

is positive definite for those values of $\gamma_i$ belonging to the interval $-1/\lambda_i^* < \gamma_i < \infty$, but the quadratic form $Q_i$ is a well-defined function of $\gamma_i$ over the more extensive interval $-1/\Delta_i^* < \gamma_i < \infty$, as is evident from representation (3.4). Further, as a function of $\gamma_i$, $Q_i$ is
strictly decreasing and strictly convex over the interval \(-1/\Delta_1^* < \gamma_1 < \infty\), and

\[
\lim_{\gamma_1 \to -1/\Delta_1^*} Q_1 = \infty, \quad \lim_{\gamma_1 \to \infty} Q_1 = 0
\]

(Harville and Fenech, 1984, Section 3). For convenience, define

\[ Q_1(-1/\Delta_1^*, \gamma_{i+1}, \ldots, \gamma_k; y) = \infty \quad \text{and} \quad Q_1(\infty, \gamma_{i+1}, \ldots, \gamma_k; y) = 0. \]

Let \( l_{k+1} = l_{k+1}(y) = Q_{k+1}/\sigma_{k+1, 1}^2 \) and \( u_{k+1} = u_{k+1}(y) = Q_{k+1}/\sigma_{k+1, 2}^2 \). Further, for any fixed value of \((\gamma_{i+1}, \ldots, \gamma_k) \in \Gamma_1\)
and for any fixed positive value of \( \sigma_{k+1}^2 \), define \( l_1 = l_1(\gamma_{i+1}, \ldots, \gamma_k, \sigma_{k+1}^2; y) \) to be the unique value of \( \gamma_1 \) that satisfies \( Q_1 = \sigma_{k+1}^2 \sigma_{k+1, 11}^{-1} r_1 \) and \( u_1 = u_1(\gamma_{i+1}, \ldots, \gamma_k, \sigma_{k+1}^2; y) \) to be the unique value of \( \gamma_1 \) that satisfies \( Q_1 = \sigma_{k+1}^2 \sigma_{k+1, 12}^{-1} r_1 \). Then, an alternative description of the 100(1-\alpha)\% confidence region \( S(y) \) is \( S(y) = \{ \sigma^2 : \sigma^2 \in Q, l_{k+1} < \sigma_{k+1}^2 < u_{k+1}, \sigma_{k+1, 11}^* < \sigma^2 < \sigma_{k+1, 11}^* u_1 (i=1, \ldots, k) \} \).

### 4.2 Special case

The upper and lower bounds \( u_1 \) and \( l_1 \) on \( \gamma_1 \) were defined as solutions to equations in \( \gamma_1 \) which are, in general, inherently nonlinear and not amenable to explicit solution. We now consider a special case where these equations can be solved explicitly.

Let \( P_{i-1}^{(0)} \) represent the value of the matrix \( P_{i-1} \) when \( \gamma_{i+1} = \ldots = \gamma_k = 0; \) that is, \( P_{i-1}^{(0)} = X_{i-1}^* (X_{i-1}^* X_{i-1}^{\ast})^{-1} X_{i-1}^* (i=1, \ldots, k+1) \). Note that the quadratic form \( y^T (1-P_0^{(0)}) y \) represents the residual sum of squares obtained from a least squares fit of the submodel \( y = X_0 \beta_0 + b_{k+1} \).
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Following Brown (1984), we define an analysis of variance for the variance components to be a partitioning

\[ y^T(I-P_0)y = y^TA_1y + \ldots + y^TA_s y, \]

where \( A_1, \ldots, A_s \) are \( n \times n \) symmetric matrices of known constants, such that

(i) \( y^TA_1y, \ldots, y^TA_s y \) are distributed independently, (ii) \( y^TA_i y/(\sigma^2 + c_i) \sim \chi^2(f_i) \) for a positive integer \( f_i \) and a scalar \( c_i \) \( (i=1, \ldots, s) \), and (iii) the scalars \( c_1, \ldots, c_s \), which are necessarily linear functions of \( \gamma_1, \ldots, \gamma_k \), are distinct. Brown showed, in effect, that an analysis of variance for the variance components exists if and only if the matrices

\[ (I-P_0)X_1X_1^T(I-P_0), \ldots, (I-P_0)X_kX_k^T(I-P_0) \]

commute in pairs, in which case the sums of squares \( y^TA_1y, \ldots, y^TA_s y \) are unique up to order.

In the Appendix, we show, by construction, that, if an analysis of variance for the variance components exists, then

\[ Q_i = \sum_{j \in I_i} y^TA_jy/c_j \quad (i=1, \ldots, k+1), \]

where \( I_1, \ldots, I_{k+1} \) represents a partitioning of the integers 1, \ldots, \( s \) into \( k+1 \) sets. We show further that, if \( s = k+1 \), then, for \( i=1, \ldots, k \),

\[ Q_i = \frac{y^T(p_i - p_{i-1})y}{1 + \sum_{j=1}^k \lambda_{ji}y_j} \]

where \( \lambda_{ji} = r_i^{-1} tr[X_j^T(p_i - p_{i-1})X_j] \) \( (j=1, \ldots, k). \)

We see that, in the special case where there exists an analysis of variance for the variance components and where, in addition, \( s = k+1 \),

\[ \lambda_i = \frac{1}{\lambda_{i1}} y^T(p_i - p_{i-1})y/(\sigma^2 + \sum^s_{k+1} \lambda^*_{i1}) - (1 + \sum_{j=i+1}^k \lambda_{ji}y_j), \]

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(4.2) \( u_i = \frac{1}{\lambda_i} \left[ y^T (p_i(0) - p_{0i}) y / \left( \frac{\sigma_i^2}{k+1} \lambda_i - \alpha_i \right) \right] - 1 + \sum_{j=1}^{k} \lambda_j y_j, \]

and that, for balanced classificatory models, our procedure for forming a confidence region reduces to the traditional procedure. Note that, in this special case, \( I \) and \( u \) are linear functions of \( y_{i+1}, ..., y_k \) and \( 1/\sigma^2 \) or, equivalently, \( \sigma^2_k \) and \( u_i \) are linear functions of \( \sigma^2_1, ..., \sigma^2_k \).

Even if an analysis of variance for all \( k+1 \) variance components does not exist, there may exist a less extensive partitioning \( y^T (I - p_k(0)) y = y^T A_k y + ... + y^T A_0 y \) such that \( y^T A_k y, ..., y^T A_0 y \) are distributed independently as distinct scalar multiples of chi-square random variables, in which case formulas (4.1) and (4.2) are still applicable, at least for \( i = k'+1, ..., k \).

5. DISCUSSION

Some modifications of the proposed procedure for obtaining a confidence region for the variance components \( \sigma^2_1, ..., \sigma^2_k \) and some considerations in its implementation are as follows:

1. The proposed procedure can be modified so as to obtain a confidence region for the variance ratios \( \gamma_1, ..., \gamma_k \). Define \( F_i = \left( \frac{r_i}{r_{k+1}/r_i} \right) \chi^2_i / \chi^2_{k+1} \) (i = 1, ..., k), where \( \chi^2_i, ..., \chi^2_{k+1} \) represent independently distributed chi-square random variables with degrees of freedom \( r_i, ..., r_{k+1} \) respectively. Take \( F_i(\lambda_i), F_i(\mu) \) (i = 1, ..., k) to be any constants such that

\[
\text{pr}[F_i(\lambda_i) < F_i(\gamma_i) \leq F_i(\mu)] = 1 - \alpha.
\]

Then, a 100(1-\( \alpha \))% confidence region for \( \gamma_1, ..., \gamma_k \) is the set

\[
S^*(\gamma) = \{ \gamma : (\gamma_1, ..., \gamma_k)^T \in \Gamma_{i-1}, \lambda_i \leq \gamma_i \leq \mu_i \text{ (i = 1, ..., k)} \}.
\]
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where \( f_1^* = f_1^*(y_1+1, \ldots, y_k; y) \) is the unique value of \( y_1 \) that satisfies
\[
\left( r_{k+1}/r_1 \right) (Q_i/Q_{k+1}) = f_1^*(u) \quad \text{and} \quad u_1^* = u_1^*(y_1+1, \ldots, y_k; y) \]
is the unique value of \( y_1 \) that satisfies \( (r_{k+1}/r_1) (Q_i/Q_{k+1}) = F_1^*(u) \).

In the special case of a balanced classificatory model and for \( \alpha_{11} = \ldots = \alpha_{k1} = 0 \), the confidence region \( S^*(y) \) simplifies to that discussed by Sahai and Anderson (1973).

If \( k \) is sufficiently large, the determination of the constants \( F_1^*(u), \) \( F_1^*(u) \) \((i=1, \ldots, k)\) may be computationally unfeasible, in which case our procedure for obtaining an exact \( 100(1-\alpha)\% \) confidence region can not be implemented. However, an approximate \( 100(1-\alpha)\% \) confidence region can be obtained by replacing \( F_1^*(u) \) and \( F_1^*(u) \) by the upper-\((1-\alpha_{12})\) and upper-\(\alpha_{11}\) points, respectively, of the marginal distribution of \( F_1^* \). It follows from Kimball's (1951) inequality that, for \( \alpha_{12} = \ldots = \alpha_{k2} = 0 \), this region is conservative; that is, its probability of coverage equals or exceeds \( 1-\alpha \).

In the special case of a balanced classificatory model and for \( \alpha_{11} = \ldots = \alpha_{k1} = 0 \), the approximate confidence region simplifies to that proposed by Broemeling (1969).

2. The proposed procedure for using the quantities \( Q_1, \ldots, Q_{k+1} \) to form a confidence region for the variance components \( \sigma_1^2, \ldots, \sigma_{k+1}^2 \) or the variance ratios \( \gamma_1, \ldots, \gamma_k \) can be modified, in an obvious way, to obtain a confidence region for the last \( k-k^*+2 \) variance components \( \sigma_{k^*}^2, \ldots, \sigma_{k+1}^2 \) or the last \( k-k^*+1 \) variance ratios \( \gamma_{k^*}, \ldots, \gamma_k \), based on the quantities \( Q_{k^*}, \ldots, Q_{k+1} \).
3. By following the approach described, for example, by Spjotvoll (1972) and Khuri (1981), the proposed confidence region for the variance components $\sigma^2_1, \ldots, \sigma^2_{k+1}$ or variance ratios $\gamma_1, \ldots, \gamma_k$ can be transformed into a generally conservative confidence region for a function of the variance components or variance ratios or, more generally, for a family of such functions. For instance, let $R_f(y)$ represent the range of a vector $f = f(\sigma^2_1, \ldots, \sigma^2_{k+1})$ of functions of variance components when the domain of $f$ is restricted to the set $S(y)$. Then, clearly, $\text{pr}[f \epsilon R_f(y)] > 1-\alpha$; that is, $R_f(y)$ is a generally conservative $100(1-\alpha)$% confidence region for $f$.

4. Often, the parameter space for the vector $\sigma^2$ is a proper subset $\Omega'$ of the set $\Omega$, rather than $\Omega$ itself. In particular, the parameter space for $\sigma^2$ may be the set $\Omega_0$.

The confidence region $S(y)$ may include values of $\sigma^2$ not belonging to $\Omega'$. Let $S'(y)$ represent the subset of $S(y)$ obtained by deleting all such values. For $\sigma^2 \in \Omega'$, $\text{pr}[\sigma^2 \epsilon S'(y)] = \text{pr}[\sigma^2 \epsilon S(y)] = 1-\alpha$. Thus, when the parameter space for $\sigma^2$ is $\Omega'$, $S'(y)$, like $S(y)$, is a $100(1-\alpha)$% confidence region for $\sigma^2$.

In the special case $\Omega' = \Omega_0$, the $100(1-\alpha)$% confidence region $S'(y)$ is obtained from $S(y)$ by deleting all values of $\sigma^2$ for which one or more of the first $k$ variance components $\sigma^2_1, \ldots, \sigma^2_k$ is negative. Expanding the set $S'(y)$ slightly, we obtain the set $S^+(y) = \{\sigma^2: \sigma^2_{k+1} > 0, l_{k+1} \leq \sigma^2_{k+1} \leq u_{k+1}, \sigma^2_{k+1} \text{ max}(l_1, 0) \leq \sigma^2_i \leq \sigma^2_{k+1} \text{ max}(u_1, 0) (i=1, \ldots, k)\}$. We have that $\text{pr}[\sigma^2 \epsilon S^+(y)]$ equals $1-\alpha$, if $\sigma^2_i > 0$ for $i=1, \ldots, k$, and is
greater than or equal to 1-\(\alpha\), otherwise, as is easily verified. Thus, when the parameter space for \(\sigma^2\) is \(Q_0\), \(S^+(y)\) is a conservative 100(1-\(\alpha\))% confidence region. Unlike \(S'(y)\), the set \(S^+(y)\) is nonempty, with probability one.

5. There will generally be more than one way to express a particular mixed or random linear model as a special case of the general mixed linear model (1.1). Consider, for example, the customary additive model for a two-way crossed classification with both factors regarded as random. We can take the elements of \(b_1\) to be the effects of the first factor or, alternatively, the effects of the second factor.

It should be noted that, except for highly structured situations, like those considered in Section 4.2, the confidence region \(S(y)\) will vary with the order in which we assign the various sets of random effects to the vectors \(b_1, \ldots, b_k\).

6. Note that, by exploiting general relationships between confidence regions and tests of hypothesis or significance, the proposed procedure for forming a confidence region can be used to test, against appropriate alternatives, a null hypothesis of the general form

\[ H_0: \sigma_1^2 = c_1, \ldots, \sigma_{k+1}^2 = c_{k+1} \quad \text{or} \quad H_0: \gamma_1 = c_1, \ldots, \gamma_k = c_k, \quad \text{where} \quad c_1, \ldots, c_{k+1} \]

represent specified constants.

Also, following Harville and Fenech (1984, Section 7), we can obtain point estimators of the variance components or variance ratios by equating the pivotal quantities \(Q_1/\sigma_{k+1}^2, \ldots, Q_{k+1}/\sigma_{k+1}^2\) or \((r_{k+1}/r_1)Q_1/Q_{k+1}\), \(\ldots, (r_{k+1}/r_k)Q_k/Q_{k+1}\) to appropriately chosen constants. In
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particular, if we equate $Q_1/\sigma_{k+1}^2, \ldots, Q_{k+1}/\sigma_{k+1}^2$ to $r_1, \ldots, r_{k+1}$, respectively, we obtain estimators which, in the special case where there exists an analysis of variance for the variance components and where $s = k+1$, simplify to the usual analysis-of-variance estimators. Alternatively, if we equate these quantities to the medians of their respective chi-square distributions, we obtain estimators that can be interpreted as the coordinates of a degenerate, single-point confidence region.

7. Let $Q = Q_1 + \ldots + Q_k$ and $r = r_1 + \ldots + r_k$, and define $P(\ell)$ and $p(u)$ to be any constants such that $P[P(\ell) < F < p(u)] = 1-\alpha$, where $F$ represents an $F$ random variable with degrees of freedom $r$ and $r_{k+1}$, respectively. Clearly, the distribution of $Q/\sigma_{k+1}^2$ is $\chi^2(r)$, and $Q$ and $Q_{k+1}$ are distributed independently. It follows that an exact $100(1-\alpha)$% confidence region for $\gamma_1, \ldots, \gamma_k$, alternative to the confidence region $S(\gamma)$, is the set $S'(\gamma)$ consisting of those values of $\gamma$ that satisfy the inequality

$$P(\ell) < (r_{k+1}/r)Q/\sigma_{k+1} < p(u).$$

It can be shown that, in the special case where $P(\ell) = 0$ (and hence where $p(u)$ is the upper-$\alpha$ point of the distribution of $F$), the confidence region $S'(\gamma)$ is the same as the exact confidence region devised by Hartley and Rao (1967, Sec. 9). We do not recommend the confidence region $S'(\gamma)$.
since, as previously indicated in the special case of the Hartley-Rao
region, it has a seemingly unappealing form and can, with high
probability, produce confidence regions of infinite volume.

8. In practice, we may want to display graphically the confidence
region $S(y)$, or when $k$ exceeds one or two, to display, for each of various
fixed values of the vector $(\sigma_{i+1}^2, \ldots, \sigma_k^2, \sigma_{k+1}^2)$ and the integer $i$, the
interval of $\sigma_i^2$ values, or perhaps the two- or three-dimensional set of
$\sigma_{i-1}^2, \sigma_i^2$ or $\sigma_{i-2}^2, \sigma_{i-1}^2, \sigma_i^2$ values, that are represented in $S(y)$. We are
then faced with the computational problem of determining the numerical
values of $l_i$ and $u_i$ corresponding to each value of $(\sigma_{i+1}^2, \ldots, \sigma_k^2, \sigma_{k+1}^2)$
and each value of $i$.

In the special case where there exists an analysis of variance
for the variance components and where $s = k+1$, this problem reduces,
in effect, to that of computing the entries in the analysis-of-variance
table. More generally, we can use the approach discussed, in the
special case $i = k$, by Harville and Fenech (1984, Section 4), to compute
the values of $L_{11}, \ldots, L_{1r_i}$ and of $\gamma_{11}, \ldots, \gamma_{1r_i}$ and to then determine the
values of $l_i$ and $u_i$ graphically or iteratively. How a series of such
determinations, involving various values of the vector $(\sigma_{i+1}^2, \ldots, \sigma_k^2, \sigma_{k+1}^2)$
and/or the integer $i$, might be accomplished most efficiently is a question
for possible investigation.
APPENDIX

Simplification of the quadratic forms

We now derive, for the special case where there exists an analysis of variance for the variance components, the simplified representations given in Section 4.2 for the quadratic forms $Q_1, \ldots, Q_k$.

Let $U_0^{(0)} = C(X_0)$, $U_1^{(0)} = C(X_1^*)^\top \cap C(X_1^*)$ (i=1,...,k), and $U_{k+1}^{(0)} = C(X_k^*)^\top$, so that, for i=1,...,k+1, $U_i^{(0)}$ represents $U_i$ when $\gamma_{i+1} = \ldots = \gamma_k = 0$. Define $M_1$ to be an $n \times r_1$ matrix whose columns form an orthonormal basis for $U_1^{(0)}$ with respect to the ordinary inner product.

Note that the columns of the matrix $M_1 = (M_0, \ldots, M_k)$ form an orthonormal basis for $C(X_1^*)$ (i=0,...,k) and that the columns of the matrix $M = (M_1, \ldots, M_{k+1})$ form an orthonormal basis for $C(X_0^*)$. Note also that, for i=0,...,k,

$$H_1^\top H_1 = H_1^\top (H_1^\top H_1)^{-1} H_1^\top = X_1^* (X_1^X_1^* - X_1^T) = p_1^{(0)}$$

and that, for i=1,...,k,

$$H_1^\top H_1 = H_1^\top (H_1^\top H_1)^{-1} H_1^\top = X_1^* (X_1^X_1^* - X_1^T) = p_1^{(0)}$$

and that, for i=1,...,k,

$$M_1^\top M_1 = M_1^\top M_1 = P_1^{(0)} - P_1^{(0)}$$

Suppose now that there exists an analysis of variance for the
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variance components. Then, the k matrices $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1 = \text{diag}[(\mathbf{M}_1, \ldots, \mathbf{M}_1)^{T}\mathbf{X}_1\mathbf{X}_1^{T}(\mathbf{M}_1, \ldots, \mathbf{M}_1), 0]$ (i=1,\ldots,k) commute in pairs

(Brown, 1984, Corollary 2), which implies that, for i=1,\ldots,k,

(A.2) $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1 = \text{diag}(\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1, \ldots, \mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1, 0, \ldots, 0),$

as we now show.

Our proof of result (A.2) is by induction. The result is clearly valid for i=1. Suppose that it is valid for i=1,\ldots,i'-1. Then, since $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1$ and $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1$ commute, implying that the ijth block of the matrix $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1$ is the same as that of $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1$, we have, for i=1,\ldots,i'-1 and j=i+1,\ldots,i', that

$\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1^{T} = 0$

and hence, in light of result (A.1), that $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1^{T} = 0$. Observing that $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1$ is symmetric, we conclude that result (A.2) is valid for i=i', which completes the proof of this result.

Now, since the matrices $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1, \ldots, \mathbf{M}_k^{T}\mathbf{X}_k\mathbf{X}_k^{T}\mathbf{M}_k$ commute in pairs, we have, in light of result (A.2), that the matrices $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1, \ldots, \mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1$ commute in pairs. Consequently, there exists an orthogonal matrix that simultaneously diagonalizes the matrices $\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1, \ldots, \mathbf{M}_k^{T}\mathbf{X}_k\mathbf{X}_k^{T}\mathbf{M}_k$; that is, there exists an orthogonal matrix $\mathbf{0}_1$ such that

$\mathbf{0}_1^{T}\mathbf{M}_1^{T}\mathbf{X}_1\mathbf{X}_1^{T}\mathbf{M}_1^{T} = \text{diag}(\lambda_{j1}, \ldots, \lambda_{jir_1})$

for some nonnegative real numbers $\lambda_{j1}, \ldots, \lambda_{jir_1}$ (j=1,\ldots,k).
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As a further consequence of result (A.2), we have that

\[ M_i^T (M_{i+1}, \ldots, M_{k+1}) = M_i^T (I + E_{s=1} \gamma_{s} X_s X_s^T ) (M_{i+1}, \ldots, M_{k+1}) = 0, \]

implying that the columns of \( M_i \), and hence those of \( M_0 \), form a basis for \( U_i \) (i=1,...,k).

For \( i=1, \ldots, k \), define

\[ w_i = (w_{i1}, \ldots, w_{ir_i})^T = (M_i 0_1)^T y, \]

define \( c_{i1}, \ldots, c_{ir_i} \) to be the distinct linear functions represented among the \( r_i \) linear functions \( 1 + E_{j=1}^k \gamma_j, \ldots, 1 + E_{j=1}^k \gamma_{j_i} \), and, for \( m=1, \ldots, r_i \), take \( t_{im} \) to be the collection of values of the index \( t \) for which \( 1 + E_{j=1}^k \gamma_{j_i} = c_{im} \); take \( f_{im} \) to be the dimension of this collection, and let \( W_{im} = t_{im} w_i^2 \).

It follows from the results of Section 3.4 that

\[ Q_i = Q_i^* = y^T M_i 0_1 (I + E_{j=1}^k \gamma_j X_j X_j^T ) (M_i 0_1)^T y \]

\[ = \sum_{m=1}^{r_i} W_{im}/c_{im} \quad (i=1, \ldots, k), \]

\[ Q_{k+1} = Q_{k+1}^* = y^T M_{k+1}^T (M_{k+1} M_{k+1}^T )^{-1} M_{k+1}^T y = y^T M_{k+1}^T M_{k+1}^T y. \]

Further we find that

\[ \sum_{i=1}^{k} r_i W_{im} + Q_{k+1} = y^T M_i^T y = y^T (I - M_0^T M_0) y = y^T (I - F_0^T (0)) y \]

and, proceeding as in Section 3.4, that \( W_{im} (i=1, \ldots, k; m=1, \ldots, r_i^*) \), \( Q_{k+1} \) are distributed independently and \( W_{im}/(c_{im}^2) \sim \chi^2(f_{im}) \), implying that \( W_{im} (i=1, \ldots, k; m=1, \ldots, r_i^*) \), \( Q_{k+1} \) are the sums of squares.
in the analysis of variance for the variance components.

Now, suppose that the analysis of variance for the variance components is such that \( s = k+1 \). Then, for \( i=1,...,k \),

\[
\lambda_{j_1} = \ldots = \lambda_{j_r} = \lambda_{j_1} \text{ for some real number } \lambda_{j_1} \text{ given by }
\]

\[
\lambda_{j_1} = r_1^{-1} \sum_{t=1}^{r_1} \lambda_{j/t} = r_1^{-1} \text{tr}(O_{j_1}^T X_j^T X_j^T M_j M_j^T O_{j_1})
\]

\[
= r_1^{-1} \text{tr}(X_j^T M_j O_{j_1}^T M_j^T X_j)
\]

\[
= r_1^{-1} \text{tr}[X_j^T (P_{j_1}^{(0)} - P_{j_{i-1}}^{(0)}) X_j] \quad (j=1,...,k)
\]

in which case

\[
Q_i = \omega_i^T \omega_i / (1+\sum_{j=1}^{k} \lambda_{j_1} y_j) = y_i^T M_i^T M_i y / (1+\sum_{j=1}^{k} \lambda_{j_1} y_j)
\]

\[
= y_i^T (P_{j_1}^{(0)} - P_{j_{i-1}}^{(0)}) y / (1+\sum_{j=1}^{k} \lambda_{j_1} y_j).
\]
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We present a general procedure for obtaining exact confidence regions for the variance components in unbalanced mixed linear models. The procedure utilizes, as pivotal quantities, quadratic forms that may depend on the variance components in a complicated way and that are distributed independently as chi-square variates. In the special case of balanced classificatory models, the pivotal quantities simplify to scalar multiples of sums of squares from the usual analysis of variance. The procedure can be easily modified so as to obtain an exact confidence region for ratios.
of variance components and can be regarded as a generalization of Wald's procedure for obtaining a confidence interval for a single variance ratio.
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