On Combining Exact and Approximative Proceedings for Testing Problems in Unbalanced Mixed Linear Models

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Abstract

A method for constructing approximative tests for arbitrary linear hypotheses on variance components in unbalanced mixed linear models is derived. The idea of cell mean models is used to derive independent and χ^2 -distributed mean squares. These modified mean squares are combined to generalized test statistics which lead to generalized fixed level tests.

1 Introduction

Unbalanced mixed linear models are widely used instruments for the analyses of situations where fixed as well as random factors influence the response. Compared to the balanced design, inference in such unbalanced models is substantially more complicated. The complication is caused by the fact that the partitioning of the total sums of squares is not unique. Consequently the usual sums of squares in general are neither stochastically independent nor distributed as multiples of χ^2 -variates. Therefore the construction of exact test procedures is only known for some very special models.

The first to construct exact tests in unbalanced variance components models was Wald (1947). Wald's idea was then further developed by Seely and El-Bassiouni (1983), but still restricted to special one—way and two—way random models and to only few hypotheses. Öfversten (1993) developed exact tests for hierarchical classifications, which then was embedded into a uniform methodology by Christensen (1996).

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A general proceeding for deriving exact tests in unbalanced random models of arbitrary structure was given by Khuri (1990). This technique leads to exact tests whenever in the balanced case the exact test for the same testing problem also exists. The method from Khuri is restricted to designs that are unbalanced on the last stage only (i.e. unequal cell frequencies), which is a common case of unbalancedness. Moreover this proceeding does not generate tests when in the corresponding balanced case nuisance parameters make exact testing impossible. A powerful tool in such cases is the generalized fixed–level test (cf. Weerahandi (1995)), which was first employed in a special unbalanced variance components model by Zhou and Mathew (1994).

Now, this paper combines Khuri's technique of deriving stochastically independent and exactly χ^2 -distributed sums of squares in unbalanced mixed linear models with the approximate testing procedure by Weerahandi. The result is an approximate testing procedure for arbitrary linear hypotheses in unbalanced mixed linear models that are unbalanced on the last stage only. A preceding work of Weimann (1998) deals with the corresponding results in the balanced case.

2 Notations in unbalanced mixed linear models

As mentioned in the introduction the unbalanced mixed linear model shall be restricted to unbalancedness on the last stage only. Then, such models can be expressed as

$$(2.1) y_{\theta} = \sum_{i=1}^{q} \gamma_{\theta_{i}(\bar{\theta}_{i})}^{(i)} + \sum_{i=q+1}^{m} g_{\theta_{i}(\bar{\theta}_{i})}^{(i)} + e_{\theta} ,$$

$$g_{\theta_{i}(\bar{\theta}_{i})}^{(i)} \sim (0, \sigma_{i}^{2}) , \quad \sigma_{i}^{2} \geq 0 \quad \text{for } i = q+1, \dots, m ,$$

$$e_{\theta} \sim (0, \sigma_{e}^{2}) , \quad \sigma_{e}^{2} > 0 ,$$

$$g_{\theta_{q+1}(\bar{\theta}_{q+1})}^{(q+1)}, \dots, g_{\theta_{m}(\bar{\theta}_{m})}^{(m)} \text{ and } e_{\theta} \text{ stochastically independent}$$

where $\gamma_{\theta_i(\bar{\theta}_i)}^{(i)}$ for $i=1\ldots,q$ are fixed effects and $g_{\theta_i(\bar{\theta}_i)}^{(i)}$ for $i=q+1,\ldots,m$ random effects. The random variable e_{θ} denotes the experimental error term. To identify a response y, the complete set of subscripts of y is given by

(2.2)
$$\theta = (_1k \dots, k_s) \quad \text{where} \quad k_j = 1, \dots, q \quad \text{for} \quad j = 1, \dots, s-1$$
 and $k_s = 1, \dots, \eta_{\omega} \quad \text{with} \quad \omega = (k_1, \dots, k_{s-1}) .$

Therefore the design is balanced with respect to the first s-1 subscripts and unbalanced with respect to the last subscript k_s .

The variables θ_i and $\bar{\theta}_i$ in the term for the i^{th} fixed respectively random effect denote the corresponding sets of rightmost † and nonrightmost bracket subscripts respectively, for $i=1,\ldots,m$, while $\psi_i=\theta_i\cup\bar{\theta}_i$ denotes the set of all subscripts of the i^{th} effect.

Since $\gamma_{\theta_1(\bar{\theta}_1)}^{(1)}$ denotes the overall mean (usually denoted by μ), which has no subscripts at all, it follows that $\theta_1 = \bar{\theta}_1 = \psi_1 = \emptyset$. We assume the existence of one variance component at minimum (i.e. $m \geq q+1$) and a usual parametrization that leads to $\psi_m = \omega$.

Let T be the set of all (s-1)-tuples defined by

$$(2.3) T = \{ \omega \mid k_i = 1, \dots, q; i = 1, \dots, s-1 \},$$

with ω given in (2.2). Be N the total number of observations, c the number of all elements in T, which is the number of all factor levels, and c_i the number of factor levels of the ith factor:

$$(2.4) \qquad c = \sum_{\omega \in T} n_{\omega} ,$$

$$c = \prod_{i=1}^{s-1} a_i ,$$

$$c_i = \prod_{k_j \in \psi_i} a_j \quad \text{for } i = 2, \dots, m \text{ and } c_1 = 1 .$$

In vector form model (2.1) can be displayed as

(2.5)
$$y = \sum_{i=1}^{q} X_{i}\beta_{i} + \sum_{i=q+1}^{m} W_{i}e_{i} + e \text{ that is}$$

$$y \sim (X\beta, \sum_{i=q+1}^{m} \sigma_{i}^{2}U_{i} + \sigma_{e}^{2}I_{N})$$

$$X_{i} \in \mathbb{R}^{N \times c_{i}} \text{ for } i = 1, \dots, q, X = (X_{1} : \dots : X_{q}), \beta = (A_{1}^{T} : \dots : \beta_{q}^{T})^{T}$$

$$W_{i} \in \mathbb{R}^{N \times c_{i}}, e_{i} \sim (0_{c_{i}}, \sigma_{i}^{2}I_{c_{i}}), U_{i} = W_{i}W_{i}^{T} \text{ for } i = q+1, \dots, m,$$

$$e \sim (0_{N}, \sigma_{e}^{2}I_{N}).$$

[†]By set of rightmost bracket subscripts $\bar{\theta}_i$ for the i^{th} effect those subscripts are meant that do not nest any other subscript of that effect. Then, the nonrightmost bracket subscripts θ_i are the complement of $\bar{\theta}_i$ with respect to set set of all subscripts ψ_i of the corresponding effect. For detail cf. Khuri (1982)

Then X_1 is the 1_N vector and β_1 is equal to the grand mean $\gamma_{\theta_1(\bar{\theta}_1)}^{(1)}$. For a given $\omega \in T$ let \bar{y}_{ω} denote the average over the corresponding y_{θ} 's with respect to the last subscript k_s :

(2.6)
$$\bar{y}_{\omega} = \frac{1}{n_{\omega}} \sum_{k_s=1}^{n_{\omega}} y_{(k_1, \dots, k_{s-1}, k_s)} , \omega \in T.$$

Let \bar{y} denote the vector consisting of the values of \bar{y}_{ω} , then

(2.7)
$$\bar{y} = Dy$$
 where $D = (F^T F)^{-1} F^T$ and $F = \bigoplus_{\omega \in T} 1_{n_\omega} = \operatorname{diag}(1_{n_{(1,\dots,1)}}, \dots 1_{n_{(a_1,\dots,a_{s-1})}})$.

Then applying formula (2.7) to model (2.1) respectively (2.5) leads to

(2.8)
$$\bar{y} = \sum_{i=1}^{q} H_i \beta_i + \sum_{i=q+1}^{m} H_i e_i + \bar{e} ,$$

where \bar{e} is defined analogously to \bar{y} in (2.6) respectively (2.7), and H_i of course can be displayed as

(2.9)
$$H_i = \begin{cases} DX_i & \text{for } i = 1, \dots, q \\ DW_i & \text{for } i = q+1, \dots, m \end{cases},$$

but also in a more constructive way as

(2.10)
$$H_i = \bigotimes_{j=1}^{s-1} L_{ij}$$
 , $L_{ij} = \begin{cases} I_{a_j} & \text{for } k_j \in \psi_i \\ 1_{a_j} & \text{for } k_j \notin \psi_i \end{cases}$ $i = 1, \dots, m$.

Since $\psi_m = \omega$ we get $H_m = I_c$. Let $H = (H_1 \cdots | H_q)$ and $\beta = (F_1, \dots, F_q^T)^T$ such that formula (2.8) can de displayed as $\bar{y} = H\beta + \sum_{i=q+1}^m H_i e_i + \bar{e}$. Then, reducing model (2.8) by invariance leads to

$$(2.11) z = Proj_{R(H)^{\perp}}\bar{y} = M\bar{y} \text{ where } M = I_c - HH^+.$$

With $A_i = H_i H_i^T$ for $i = q + 1, \ldots, m$ the reduced model can be displayed as

(2.12)
$$z \sim \left(0, \sum_{i=q+1}^{m} \sigma_i^2 V_i + \sigma_e^2 K\right) \text{ where } V_i = M A_i M \text{ for } i = q+1, \dots, m$$
$$K = M \left[\bigoplus_{\omega \in T} \left(\frac{1}{n_\omega}\right) \right] M,$$

which has to be proved:

$$E[z] = E[M] = MH\beta = (M-HH^+)H\beta = 0$$

$$Cov[z] = Cov[M] = MCov \left[\sum_{i=q+1}^{m} H_i e_i + \bar{e}\right] M$$

$$= M \left\{\sum_{i=q+1}^{m} \sigma_i^2 H_i H_i^T + \sigma_e^2 \bigoplus_{\omega \in T} \left(\frac{1}{n_\omega}\right)\right\} M$$

$$= \sum_{i=q+1}^{m} \sigma_i^2 M A_i M + \sigma_e^2 M \left[\bigoplus_{\omega \in T} \left(\frac{1}{n_\omega}\right)\right] M$$

$$= \sum_{i=q+1}^{m} \sigma_i^2 V_i + \sigma_e^2 K.$$

Remark 2.1. A certain \bar{y}_{ω} has a corresponding row in A_i . This row is identical with n_{ω} rows of U_i since $\gamma_{\theta_1(\bar{\theta}_1)}^{(1)}, \ldots, \gamma_{\theta_q(\bar{\theta}_q)}^{(q)}, g_{\theta_{q+1}(\bar{\theta}_{q+1})}^{(q+1)}, \ldots, g_{\theta_m(\bar{\theta}_m)}^{(m)}$ are not affected by averaging over the last subscript.

It can easily be verified that V_{q+1}, \ldots, V_m commute (i.e. $V_i V_j = V_j V_i$ for $i \neq j$). Therefore an orthogonal matrix of order $c \times c$ exists that diagonalizes V_{q+1}, \ldots, V_m simultaneously:

$$(2.13) QV_iQ^T = D_i , i = q+1, \dots, m,$$

where D_i is a diagonal matrix. This statement is proven in the appendix in Corollary 5.1 and an algorithm for constructing Q is given.

Let vector u be defined by

$$(2.14) u = Qz.$$

Then we have from (2.12) and (2.14)

(2.15)
$$E[u] = Q E[z] = 0$$
(2.16)
$$Cov[u] = Q Cov[z]Q^{T}$$

$$= \sum_{i=q+1}^{m} \sigma_{i}^{2} Q V_{i} Q^{T} + \sigma_{e}^{2} Q K Q^{T}$$

$$= \bigoplus_{i=q+1}^{m} \delta_{i} I_{m_{i}} + \sigma_{e}^{2} G , G = Q K Q^{T}$$

where δ_i (cf. (2.17)) and m_i (cf. (2.19)) can be derived from the embedded balanced model, that is model 2.1 with $n_{\omega} = 1$ for all $\omega \in T$: δ_i is the expectation of the i^{th} mean square (of the embedded balanced model) and in a formal notation it is given by

(2.17)
$$\delta_i = \sum_{j \in \varphi_i} b_j \sigma_j^2 \quad , \quad \text{with } \varphi_i = \{ j \mid q+1 \le j \le m \ , \ \psi_i \subseteq \psi_j \} \ ,$$

with b_j from (5.7).

Since then V_{q+1}, \ldots, V_m with $V_m = M$ is a basis of a commutative and quadratic subspace of the space of symmetric matrices (the embedded model is a balanced model of ANOVA-type) with $g_{\theta_m(\bar{\theta}_m)}^{(m)}$ taking the role of the experimental error term, there exists a basis P_{q+1}, \ldots, P_m

of orthogonal projectors of the same subspace. The basis transform is given by the matrix $\Phi = (\varphi_j)_{ij}$ with

(2.18)
$$V_i = \sum_{j=q+1}^m \varphi_{ij} P_j \text{ for } i = q+1, \dots, m.$$

Moreover, P_1, \ldots, P_m are the projectors of the sums of squares according to the embedded balanced model. Then m_i is the rank of projector P_i :

$$(2.19)$$
 $m_i = \text{Rank}(P_i)$, $i = 1, ..., m$.

This is verified in detail in Khuri (1998). Since many balanced models are made explicit in Hartung *et al.* (1997) the derivation of m_i , δ_i , and P_i in general is straightforward.

Now, if G were not present in (2.16), u could easily be used to construct exact tests concerning $\sigma_{q+1}^2, \ldots, \sigma_m^2$, since then the components of u would be stochastically independent. In the balanced case with $n_{\omega} = n_0$ for all $\omega \in T$ we have $K = I_c/n_0$ and because Q can be constructed as a orthonormal matrix then G is a multiple of an identity matrix, too. Then (2.16) coincides with the variance—covariance matrix of y_{θ} in the balanced case, except for the factor $1/n_0$ of variance component σ_e^2 which is caused by averaging over the last subscript.

3 Derivation of exact tests

The technique of deriving exact tests in the case random models with unbalancedness on the last stage only, was introduced by Khuri (1990). Khuri's method needs a further weak assumption on the sample size (cf.(3.3)), which should be fulfilled in most cases.

The residual sum of squares for the unbalanced model (2.1) is given by

$$(3.1) SS(e) = y^T R y , R = I_N - F F^+ ,$$

where F is the block-diagonal matrix defined in (2.7). From Khuri (1990) we have the following Lemma:

Lemma 3.1.

1. R is idempotent of rank N-c, where N and c are defined in (2.4).

2.
$$DR = 0$$
, where D is given in (2.7).

3.
$$RH_i = 0$$
 for $i = 1, ..., m$, where $H_1, ..., H_m$ are given in (2.9) resp. (2.10).

With Lemma 3.1 R can be decomposed to

$$(3.2) R = C\Lambda C^T,$$

where C is an orthogonal and Λ a diagonal matrix. Furthermore the diagonal of Λ consists of N-c ones and c zeroes. With the assumption of

$$(3.3) N > 2c - 1$$

 Λ can be partitioned such that

(3.4)
$$\Lambda = \operatorname{diag}(I_{c-\xi}, I_{N-2c+\xi}, 0_c) , \quad \xi = \sum_{i=1}^{p} m_i ,$$

with m_i from (2.19). Assume that C is partitioned analogously to Λ , that is

(3.5)
$$C = (\mathcal{Q}C_2|C_3) \text{ , with } C_1 \in \mathbb{R}^{N \times (c-\xi)},$$

$$C_2 \in \mathbb{R}^{N \times (N-2c+\xi)},$$

$$C_3 \in \mathbb{R}^{N \times c}.$$

Define

(3.6)
$$\phi = u + (\lambda_{max} I_{c-\xi} - G)^{1/2} C_1^T y,$$

where λ_{max} is the largest eigenvalue of G defined in (2.16). Let ϕ be partitioned as $\phi = (\phi_{q+1}^T | \dots | \phi_m^T)^T$ where ϕ_i is of order $m_i \times 1$. Then we have analogously to a Lemma given by Khuri (1990):

Lemma 3.2.

- 1. $E[\phi_i] = 0 \text{ for } i = q + 1, \dots, m$.
- 2. $\phi_{q+1}, \ldots, \phi_m$ are independently distributed as normal vectors and the variance-covariance matrix of ϕ_i is given by

$$\operatorname{Var}\left[\phi_{i}\right] = \left(\delta + \lambda_{max}\sigma_{e}^{2}\right)I_{m_{i}}, \ i = q + 1, \dots, m,$$

where δ_i is given in (2.17).

3. $\phi_{q+1}, \ldots, \phi_m$ are independent of $SS_2(e) = y^T C_2 C_2^T y$, which is the portion of the residual sum of squares SS(e) corresponding to matrix C_2 in formula (3.5).

This Lemma leads directly to the following Corollary (also given by Khuri (1990)), that will be used to obtain independently χ^2 -distributed sums of squares in the unbalanced case.

Corollary 3.3.

Let $SS_i = \phi_i^T \phi_i$, where ϕ is given in (3.6). Then,

- 1. SS_{q+1}, \ldots, SS_m are independent.
- 2. $SS_i/(\delta_i + \lambda_{max}\sigma_e^2)$ is distributed as a central χ^2 -variate with m_i degrees of freedom (i = q + 1, ..., m).
- 3. SS_{q+1}, \ldots, SS_m are independent of $SS_2(e)/\sigma_e^2$, which has the central χ^2 -distribution with $N-2c+\xi$ degrees of freedom.

With modified mean squares $MS_i = SS_i/m_i$ for $i = q+1, \ldots, m$ and $MS_2(e) = SS_2(e)/(N-2c+1)$ F-tests can be constructed in the traditional way, such that a ratio of two mean squares is exactly central F-distributed under a certain null hypothesis.

This technique of course can only be applied for a few hypotheses, for example for testing if a single variance component is zero. But, even in such simple cases, sometimes exact testing with traditional F-tests is impossible. Moreover arbitrary linear hypotheses in general will not be testable with an exact F-test and, as a matter of course, there are no hypotheses that are exactly testable in the unbalanced model if they are not exactly testable in the corresponding balanced model.

4 Approximate tests

Now the generated independent χ^2 -distributed random variables $SS_{q+1}, \ldots, SS_m, SS_2(e)$ are used to construct approximate tests on arbitrary linear hypotheses.

Let $\sigma^2 = (\sigma_{q+1}^2, \dots, \sigma_m^2, \sigma_e^2)^T \in \mathbb{R}^{m-q+1}$ be the vector of all variance components. Then, as demonstrated in Weimann (1998), general linear hypotheses of the form

$$(4.1) H_0^I: d^T\sigma^2 = c_0 vs. H_1^I: d^T\sigma^2 \neq c_0 ,$$

$$H_0^{II}: d^T\sigma^2 \leq c_0 vs. H_1^{II}: d^T\sigma^2 > c_0 ,$$

$$H_0^{III}: d^T\sigma^2 \geq c_0 vs. H_1^{III}: d^T\sigma^2 < c_0 ,$$

where $d \in \mathbb{R}^{m-q+1}$ and $c_0 \in \mathbb{R}$ can be tested with an approximate generalized fixed level test.

As a preliminary step the vector of parameters has to be devided into one parameter, that takes the role of the parameter of interest and the vector of the other parameters, which in the context of the generalized fixed level test will function as nuisance parameters. The parameter of interest is basically arbitrary, but has to occur in H_0 , that is, the corresponding d_i must be nonzero.

Therefore the hypotheses (4.1) has to be transformed, leaving an arbitrary single parameter (the parameter of interest) on the left side of the special null hypothesis:

$$H_{0}^{I}: \quad \sigma_{i}^{2} = \frac{1}{d_{i}} \left(c_{0} - \sum_{j \neq i} d_{j} \sigma_{j}^{2} \right) \quad \text{vs.} \quad H_{1}^{I}: \quad \sigma_{i}^{2} \neq \frac{1}{d_{i}} \left(c_{0} - \sum_{j \neq i} d_{j} \sigma_{j}^{2} \right) \quad ,$$

$$(4.2) \quad H_{0}^{II}: \quad \sigma_{i}^{2} \leq \frac{1}{d_{i}} \left(c_{0} - \sum_{j \neq i} d_{j} \sigma_{j}^{2} \right) \quad \text{vs.} \quad H_{1}^{II}: \quad \sigma_{i}^{2} > \frac{1}{d_{i}} \left(c_{0} - \sum_{j \neq i} d_{j} \sigma_{j}^{2} \right) \quad ,$$

$$H_{0}^{III}: \quad \sigma_{i}^{2} \geq \frac{1}{d_{i}} \left(c_{0} - \sum_{j \neq i} d_{j} \sigma_{j}^{2} \right) \quad \text{vs.} \quad H_{1}^{III}: \quad \sigma_{i}^{2} < \frac{1}{d_{i}} \left(c_{0} - \sum_{j \neq i} d_{j} \sigma_{j}^{2} \right) \quad ,$$

Now by definition σ_i^2 takes the role of the parameter of interest and all other σ_j^2 $(j \neq i)$, collected in the vector $\tilde{\sigma}^2 := (\sigma_1^2, \dots, \sigma_{i-1}^2, \sigma_{i+1}^2, \dots, \sigma_{m-q}^2)^T$ function as nuisance parameters.

For the problem of testing an arbitrary linear hypothesis of variance components as in (4.1) resp. (4.2) consider the following random variable (cf. Weimann (1998))

$$(4.3) T(Y, y, \sigma^2) = \frac{\sum_{l \in L} \beta_l \cdot (\delta_l + \lambda_{max} \sigma_e^2) \frac{ss_l}{SS_l} + \beta_0 c_0}{\alpha_0 A \frac{ss_i}{SS_i} + \sum_{k \in K} \alpha_k \cdot (\delta_k + \lambda_{max} \sigma_e^2) \frac{ss_k}{SS_k}},$$

where ss_l is the observed value of SS_l , $K, L \subseteq \{q+1, \ldots, i-1, i+1, \ldots, m, m+1\}$, $SS_{m+1} = SS_2(e)$ from Lemma 3.2, $\delta_{m+1} = 0$, constants $\alpha_k, \beta_l \in \mathbb{R}$ and

$$(4.4) A = \delta_i + \lambda_{max} \sigma_e^2 - \sigma_i^2 \varphi_{ii} + \varphi_{ii} \left[\frac{1}{d_i} \left(c_0 - \sum_{j \neq i} d_j \sigma_j^2 \right) \right] ,$$

with φ_{ii} an element of the basis transform defined in (2.18), such that

$$(4.5) \alpha_0 A + \sum_{k \in K} \alpha_k \cdot (\delta_k + \lambda_{max} \sigma_e^2) = \sum_{l \in L} \beta_l \cdot (\delta_l + \lambda_{max} \sigma_e^2) + \beta_0 c_0 ,$$

and all added terms shall be nonnegative:

(4.6)
$$\alpha_k \cdot (\delta_k + \lambda_{max} \sigma_e^2) \geq 0 \quad \forall \quad k \in K \quad , \quad \alpha_0 A \geq 0 ,$$
$$\beta_l \cdot (\delta_l + \lambda_{max} \sigma_e^2) \geq 0 \quad \forall \quad l \in L \quad , \quad \beta_0 c_0 \geq 0 .$$

Lemma 4.1. The random variable $T(Y, y, \sigma^2)$ from (4.3) with assumptions (4.5) and (4.6) possesses the three properties of a generalized test variable, that is

- 1. the observed value of T is independent of any parameter,
- 2. the probability distribution of T under H_0 is free of the nuisance parameters $\tilde{\sigma}_i^2$,
- 3. $\Pr(T \leq t | \sigma_i^2)$ is a monotonic function of σ_i^2 for any given t.

1. The observed value of T

$$t_{obs} = T(y, y, \sigma^2) \stackrel{(4.3)}{=} \frac{\sum_{l \in L} \beta_l \cdot (\delta_l + \lambda_{max} \sigma_e^2) + \beta_0 c}{\alpha_0 A + \sum_{k \in K} \alpha_k \cdot (\delta_k + \lambda_{max} \sigma_e^2)} \stackrel{(4.5)}{=} 1$$

is constant and therefore especially independent of any parameters.

2. Since α_k, β_l and s_i are constant and due to Corollary 3.3

$$\sum_{k \in K} \alpha_k \cdot (\delta_k + \lambda_{max} \sigma_e^2) \frac{s s_k}{S S_k} \quad \text{and} \quad \sum_{l \in L} \beta_l \cdot (\delta_l + \lambda_{max} \sigma_e^2) \frac{s s_l}{S S_l}$$

are linear combinations of independent $1/\chi^2$ -expressions, free of any unknown parameter. β_0 and c are constant. Finally, for the left term in the denominator of T in (4.3) we get

$$(4.7) \alpha_0 A \frac{ss_i}{SS_i} = \alpha_0 ss_i \frac{A}{(\delta_i + \lambda_{max}\sigma_e^2)} \frac{(\delta_i + \lambda_{max}\sigma_e^2)}{SS_i} \stackrel{H_0^I}{=} \alpha_0 ss_i \frac{(\delta_i + \lambda_{max}\sigma_e^2)}{SS_i} ,$$

also an $1/\chi^2$ -expression, which at least under the assumption of H_0^I is free of nuisance parameters (cf. Corollary 3.3).

3. By construction the parameter of interest σ_i^2 in T only appears in $\alpha_0 A \cdot ss_i/SS_i$ in the denominator of (4.3), since all other possibly appearing σ_i^2 belong to $1/\chi^2$ -variates. With respect to the vector of variance components σ^2 we have

$$T(Y, y, \sigma^2) \propto \frac{q_1}{q_2 \frac{A}{\delta_i + \lambda_{max} \sigma_e^2} + q_3}$$

Because of (4.6) it follows that $q_1, q_2, q_3 \in \mathbb{R}_0^+$, and for that reason T is stochastically increasing in δ_i and therefore also in σ_i^2 , since δ_i is the expected value of the i^{th} mean square in the embedded balanced model.

With 1., 2. and 3. T is a generalized test variable.

So, the generalized p-values for the three testing problems (4.2) are given for

$$(4.8) H_0^I: p = 2 \cdot \min \left(\Pr(T(Y, y, \sigma^2) \ge 1 \mid H_0^I) , \Pr(T(Y, y, \sigma^2) \le 1 \mid H_0^I) \right)$$

$$(4.8) H_0^{II}: p = \Pr(T(Y, y, \sigma^2) \ge 1 \mid d^T \xi = c)$$

$$(4.8) H_0^{III}: p = \Pr(T(Y, y, \sigma^2) \le 1 \mid d^T \xi = c) ,$$

and the generalized fixed-level test of level α is given by the rule

"reject
$$H_0$$
 if $p \leq \alpha$ ".

For a detailed description of the theory of generalized fixed level tests cf. Weimann (1998).

5 Appendix

Corollary 5.1. Let A_1, \ldots, A_n be symmetric $k \times k$ matrices. Assume all A_i to be pairwise commutative (i.e. $A_iA_j = A_jA_i \ \forall \ i, j = 1, \ldots, n$), then, an orthogonal matrixQ exists, such that Q^TA_iQ is a diagonal matrix for all $i = 1, \ldots, n$.

Proof. For n = 2: cf. Graybill (1983, p. 406ff). For n > 2: complete induction.

A)
$$n = 1$$

 A_1 is a symmetric Matrix. Therefore matrices Q_1 and D_1 exist, such that

$$Q_1^T A_1 Q_1 = D_1 ,$$

where Q_1 is orthogonal and D_1 diagonal. So, for n=1 the Corollary is proven.

$$\underline{\mathrm{B}})\ n \to n+1$$

Let Q_n be given such that:

$$(5.1) Q_n^T A_i Q_n = D_i \quad \forall \ i = 1, \dots, n ,$$

where Q_n is orthogonal and D_i is diagonal for $i=1,\ldots,n$. In fact D_i can be written as

where $\lambda_{i1}, \ldots, \lambda_{il_i}$ are the distinct characteristic roots of A_i . If n_{ij} is the multiplicity of characteristic root λ_{ij} then the identity matrix I_{ij} is of order $n_{ij} \times n_{ij}$. Let

$$(5.2) C := Q_n^T A_{n+1} Q_n .$$

Then with (5.1), the commutativity of A_i for $i \in \{1, ..., n\}$ and the orthogonality of Q_n it holds:

(5.3)
$$D_{i}C = Q_{n}^{T}A_{i}Q_{n}Q_{n}^{T}A_{n+1}Q_{n} = Q_{n}^{T}A_{i}A_{n+1}Q_{n}$$
$$= Q_{n}^{T}A_{n+1}A_{i}Q_{n} = Q_{n}^{T}A_{n+1}Q_{n}Q_{n}^{T}A_{i}Q_{n} = CD_{i}.$$

By Partitioning of C it follows especially from (5.3) with $D_nC=CD_n$

$$\begin{bmatrix} \lambda_{n1}I_{n1} & 0 & \cdots & 0 \\ 0 & \lambda_{n2}I_{n2} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \lambda_{nl_n}I_{nl_n} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1n} \\ C_{21} & C_{22} & \cdots & C_{2n} \\ \vdots & \vdots & & \vdots \\ C_{n1} & C_{n2} & \cdots & C_{nn} \end{bmatrix}$$

$$= \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1n} \\ C_{21} & C_{22} & \cdots & C_{2n} \\ \vdots & \vdots & & \vdots \\ C_{n1} & C_{n2} & \cdots & C_{nn} \end{bmatrix} \begin{bmatrix} \lambda_{n1}I_{n1} & 0 & \cdots & 0 \\ 0 & \lambda_{n2}I_{n2} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \lambda_{nl_n}I_{nl_n} \end{bmatrix}.$$

This implies $C_{rs} = 0$ for $r \neq s$ since $\lambda_{nr} \neq \lambda_{ns}$ for $r \neq s$ and C only consists of diagonal blocks. As A_{m+1} is symmetric, C from (5.2) is symmetric too, and therefore also C_{jj} . This once again implies the existence of matrices \widetilde{Q}_j and D_j , such that

(5.4)
$$\widetilde{Q}_j^T C_{jj} \widetilde{Q}_j = D_j \text{ for all } j = 1, \dots, l,$$

where the \widetilde{Q}_j are orthogonal and D_j diagonal. Let

$$\widetilde{Q} := \bigoplus_{i=1}^{l} \widetilde{Q}_i = \operatorname{diag}(\widetilde{Q}_1, \dots, \widetilde{Q}_l),$$

then according to (5.4) \widetilde{Q} is orthogonal and for $i \in 1, \ldots, n$ it follows

(5.5)
$$\widetilde{Q}^{T}Q_{n}^{T}A_{i}Q_{n}\widetilde{Q} \stackrel{(5.1)}{=} \widetilde{Q}^{T}D_{i}\widetilde{Q} = D_{i} \text{ for all } i = 1, \dots, n$$

$$\widetilde{Q}^{T}Q_{n}^{T}A_{n+1}Q_{n}\widetilde{Q} \stackrel{(5.2)}{=} \widetilde{Q}^{T}C\widetilde{Q} = D^{*} ,$$

where even D^* is diagonal (cf. (5.4)). Finally let

$$Q_{n+1} := Q_n \widetilde{Q} ,$$

so Q_{n+1} according to (5.4) diagonalizes A_1, \ldots, A_n as well as A_{n+1} simultaneously. Q_{n+1} is orthogonal, as Q_n and \widetilde{Q} are orthogonal. With A) and B) Corollary 5.1 is proven.

Remark 5.2. Corollary 5.1 even holds in the opposite direction: if there exists an orthogonal matrix P that diagonalizes symmetric matrices A_1, \ldots, A_n simultaneously, then the set of A_i commutes. (cf. Graybill (1983, p. 408)).

5.1 Construction of the diagonalization matrix

Of course Corollary 5.1 can be used to construct the diagonalization matrix Q. Since this would take some effort in programming, we give a straighter method to construct Q:

For the construction of Q, one should first write down the expressions for the P_i matrices using the following formula:

(5.6)
$$P_{i} = \sum_{j=1}^{m} \frac{\lambda_{ij}}{b_{j}} A_{j} , \quad i = q+1, \dots, m ,$$

with $A_j = H_j H_j^T$ (cf. formula (2.10)), λ_{ij} is -1, 0 or 1 which is the coefficient of the j^{th} admissible mean in the i^{th} component of the balanced model (cf. Khuri (1982)) and b_j is given by

(5.7)
$$b_{j} = \begin{cases} \prod_{k_{l} \notin \psi_{j}} a_{l}, & \text{if } \psi_{j} \neq \omega \\ 1, & \text{if } \psi_{j} = \omega \end{cases}$$
 $j = 1, \dots, s-1,$

where a_l , s and ω are introduced in (2.2) and $\psi_j = \theta_j \cup \bar{\theta_j}$ is defined as before.

Now, let Q_i be the matrix whose rows are orthonormal and form a basis for the rows of P_i . The rows of Q_i are in fact orthonormal eigenvectors of the idempotent matrix P_i which correspond to the eigenvalue 1 of P_i . These are easily obtained using, for example, the EIGEN subroutine in PROC IML of SAS. Note that Q_i is not unique, and hence Q_i is not unique. Then diagonalization matrix Q_i is given by $Q_i = (Q_{i+1}^T | \dots | Q_m^T)^T$. This is the result of a Lemma given by Khuri (1998, p.123f).

5.2 An alternative principle of construction

An alternative proceeding (via singular value decomposition instead of eigenvalue detection) which can be directly transferred into program code of any computer language is given by the following:

- 1. Singular value decomposition of A_1 : Compute $Q^T A_1 Q = D$ with R orthogonal and D diagonal.
- 2. Let $C := Q^T A_n Q$.
- 3. C consists of diagonal blocks and can be displayed as $C = \operatorname{diag}(C_1, \ldots, C_l)$.
- 4. Singular value decomposition of C_i : Compute $\widetilde{Q}_i^T C_i \widetilde{Q}_i = D_i$ with \widetilde{Q}_i orthogonal and D_i diagonal for all $i = 1, \ldots, l$
- 5. Let $\widetilde{Q} := \operatorname{diag}(\widetilde{Q}_1, \dots, \widetilde{Q}_{\rho}).$
- 6. Let $P := Q \cdot \widetilde{Q}$
- 7. If the diagonalization of all A_i is not yet completed, go on with item 3 and Q := P, $C := Q^T A_{n+1} P$; otherwise matrix P = Q for simultaneously diagonalization is given.

As noted above this proceeding is the consequence of using Corollary 5.1.

6 Examples

Example 1

The following example is taken from Khuri and Littell (1987) and deals with variation in fusiform rust in Southern pine tree plantations. Trees with female parents from different families were evaluated in several test locations. The data from five families and four test locations are extracted, while the male parents are disregarded for purpose of illustration.

Table 1: Proportions of symptomatic trees from five families and four test locations

Test	Family number							
number	288	352	19	141	60			
	.804	.734	.967	.917	.850			
34	.967	.817	.930					
01	.970	.833	.889					
		.304						
	.867	.407	.896	.952	.486			
35	.667	.511	.717		.467			
55	.793	.274						
	.458	.428						
	.409	.411	.919	.408	.275			
36	.569	.646	.669	.435	.256			
00	.715	.310	.669	.500				
	.487		.450					
	.587	.394	.928	.367	.525			
37	.538	.428	.855					
01	.961		.655					
	.300		.800					

The number of plots in each family × test combination ranged from one to four. Proportions of symptomatic trees in each plot are recorded in Table 1.

Here α_i is the random effect of the i^{th} family, b_j the random effect of the j^{th} test location and $(ab)_{ij}$ denotes the random interaction term of the i^{th} family and the j^{th} test location. The overall mean ist given by μ and the error term by e_{ijk} .

For the data in Table 1 an unbalanced 2–way crossed classification model with random effects is used:

(6.1)
$$y_{ijk} = \mu + a_i + b_j + (ab)_{ij} + e_{ijk} ,$$

$$i = 1, \dots, r , j = 1, \dots, s , k = 1, \dots, \eta_{i,j)} ,$$

$$a_i \sim (0, \sigma_a^2) , b_j \sim (0, \sigma_b^2) , (ab)_{ij} \sim (0, \sigma_{ab}^2) , e_{ijk} \sim (0, \sigma_e^2) ,$$

$$a_i, b_i, (ab)_{ij} \text{ and } e_{ijk} \text{ stochastically independent} .$$

With section 2 the following results are easily obtained:

Moreover we have

$$c = r \cdot s = 20$$
 , $N = \sum_{\omega \in T} n_{\omega} = 53$, $\omega = (i, j)$, $\theta = (i, j, k)$, $q = 1$, $m = 4$,

and the basis transformation matrix Φ from (2.18) and matrix Λ , used for constructing the diagonalization matrix Q in formula (5.6), are given by

$$\Phi = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & s & 0 & 0 \\ 0 & 0 & r & 0 \\ 0 & 1 & 1 & 1 \end{pmatrix} \quad , \quad \Lambda = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 1 & -1 & -1 & 1 \end{pmatrix} .$$

Using SAS/IML the following results are obtained (cf. section 3):

$$SS(e) = 0.846, \ \lambda_{max} = 1$$

 $SS_2(e) = 0.256, \ SS_a = 0.203, \ SS_b = 0.628, \ SS_{ab} = 0.168$

Then the generalized p-value for

(6.2)
$$H_0: \sigma_a^2 = \sigma_b^2 \quad \text{vs.} \quad H_1: \sigma_a^2 \neq \sigma_b^2$$

according to (4.8) can be computed as

(6.3)
$$p = 2 \cdot \min\{\Pr(T(Y, y, \sigma) > 1), \Pr(T(Y, y, \sigma) < 1)\}$$

with

(6.4)
$$T(Y, y, \sigma) = \frac{r \cdot (s\sigma_a^2 + \sigma_{ab}^2 + \lambda_{max}\sigma_e^2) \frac{ss_a}{SS_a} + s \cdot (\sigma_{ab}^2 + \lambda_{max}\sigma_e^2) \frac{ss_{ab}}{SS_{ab}}}{s \cdot (r\sigma_a^2 + \sigma_{ab}^2 + \lambda_{max}\sigma_e^2) \frac{ss_b}{SS_b} + r \cdot (\sigma_{ab}^2 + \lambda_{max}\sigma_e^2) \frac{ss_{ab}}{SS_{ab}}}$$

and the result returned by 50.000 simulations is

$$p = 0 .272$$

such that the difference between the two variance components is not significant at the 5%-level.

Example 2

The second example is taken from Zhou and Mathew (1994) and concerns an experiment to compare a new tube (NT) with a control tube (CT) to be used for firing ammunition from tanks. The problem is to test is tube—to—tube variability is less for the new tube compared to the control tube. Twenty NT's and twenty CT's were randomly selected for the experiment with four tanks each for mounting the NT's and CT's. Five NT's were mounted on each of four tanks, and five CT's were mounted on each of the four other tanks. Three rounds were fired from each tube, and the observations consisted of a miss distance (the unit used was 6.400 mils per 365 degrees).

Table 2: Miss distances for the tube-to-tube variability experiment

$\overline{\text{Tank } i}$	CT_{i1}	CT_{i2}	CT_{i3}	CT_{i4}	CT_{i5}	NT_{i1}	NT_{i2}	NT_{i3}	NT_{i4}	NT_{i5}
i = 1	2.76	1.83	1.60	1.53	2.20	1.92	1.98	2.28	1.52	1.61
	2.10	1.65	1.56	2.29	2.59	1.77	1.56	1.90	1.82	1.48
	1.61		1.73	2.06	1.91		1.83	2.10	1.79	
i=2	1.35	1.15	1.71	1.70	1.26	1.70	1.61	1.78	1.60	1.69
	1.64	1.83	1.63	1.26	1.69	1.82	1.71	1.73	1.65	1.72
	1.56	1.92		1.64		1.65				1.76
i=3	1.28	1.65	1.94	1.72	1.81	1.79	1.64	1.84	1.80	1.73
		1.76	1.86	1.56	2.13	1.39	1.88	1.67	1.49	1.83
		1.81	2.00	1.91	1.86	1.52	1.60	1.64	1.92	1.79
i=4	1.64	1.77	1.01	1.78	1.27	1.60	1.88	1.77	1.46	2.10
	1.80	1.63	1.63	1.86	1.38	1.63	1.60	1.56	1.29	1.46
	1.89	1.51	1.46		1.55		1.61	1.62	1.72	1.60

Originally the data set was balanced. For purpose of demonstration some observations are assumed to be missing. Therefore the design is unbalanced.

Let CT_{ij} and NT_{ij} respectively denote the j^{th} CT and the j^{th} NT mounted on the i^{th} tank $(i=1,\ldots,r;\ j=1,\ldots,s)$. From the above it is clear, that r=4 and s=5. The measurements (the miss distances) corresponding to each CT_{ij} and NT_{ij} are given in Table 2. Let y_{ijk} and z_{ijk} respectively denote the k^{th} observation corresponding to CT_{ij} and NT_{ij} , α_i denote the effect due to the i^{th} tank on which a CT was mounted, γ_i denote the effect due to CT_{ij} , and d_{ij} denote the effect due to NT_{ij} . The 2-way hierarchical models with mixed effects to be used for analyzing the data in Table 2 are

$$(6.5) y_{ijk} = \mu_1 + \alpha_i + b_{ij} + e_{ijk} ,$$

(6.6)
$$z_{ijl} = \mu_2 + \gamma_i + d_{ij} + f_{ijl},$$
with $i = 1, \dots, r, j = 1, \dots, s$

$$k = 1, \dots, \eta^y_{(i,j)}, l = 1, \dots, \tilde{\eta}_{(i,j)}$$

where μ_1 and μ_2 are the overall means and e_{ijk} and f_{ijl} denote random–error terms. The tank effects α_i and γ_i (i = 1, ..., r) are fixed unknown parameters. We also assume that

$$b_{ij} \sim N(0, \sigma_b^2)$$
 , $d_{ij} \sim N(0, \sigma_d^2)$, $e_{ijk} \sim N(0, \sigma_e^2)$, $f_{ijl} \sim N(0, \sigma_e^2)$,

and all the random variables are independent. Note that models (6.5) and (6.6) are unbalanced two-way nested models with mixed effects.

Once again with section 2 the following results for both models are easily obtained:

In this example we have

$$c = r \cdot s$$
, $\omega = (i, j)$, $\theta = (i, j, k)$, $q = 2$, $m = 3$,

the number of observations is given by

$$N^y = \sum_{\omega \in T} n_\omega^y = 55 \; , \; N^z = \sum_{\omega \in T} n_\omega^z = 54 \; ,$$

and matrix Λ , used for constructing the diagonalization matrix Q in formula (5.6), is given by

$$\Lambda = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -1 & 1 \end{pmatrix} .$$

Using SAS/IML the following results are obtained (cf. section 3) for the CT's from model (6.2):

$$SS^{CT}(e) = 2.302, \ SS_2^{CT}(e) = 0.567, \ SS_b^{CT} = 1.781, \ \lambda_{max}^{CT} = 0.\overline{8},$$

and for the NT's from model (6.3):

$$SS^{NT}(e) = 0.913, \ SS_2^{NT}(e) = 0.570, \ SS_d^{NT} = 0.223, \ \lambda_{max}^{NT} = 0.5.$$

To asses whether tube–to–tube dispersion is less among the NT's compared to the CT's, we have to test the hypothesis

(6.7)
$$H_0: \sigma_b^2 \le \sigma_d^2 \quad \text{vs.} \quad \sigma_b^2 > \sigma_d^2$$
.

The generalized p-value for testing the hypothesis in (6.7) according to (4.8) is given by

(6.8)
$$p = \Pr((Y, Z, y, z, \sigma) \ge 1) | \sigma_b^2 = \sigma_d^2)$$

with

(6.9)
$$T(Y, Z, y, z, \sigma) = \frac{(\sigma_d^2 + \lambda_{max}^{NT} \cdot \sigma_f^2) \frac{s s_d^{NT}}{S S_d^{NT}} + \lambda_{max}^{CT} \cdot \sigma_e^2 \frac{s s_2^{CT}(e)}{S S_2^{CT}(e)}}{(\sigma_d^2 + \lambda_{max}^{CT} \cdot \sigma_e^2) \frac{s s_b^{CT}}{S S_b^{CT}} + \lambda_{max}^{NT} \cdot \sigma_f^2 \frac{s s_2^{NT}(e)}{S S_2^{NT}(e)}}$$

and the result returned by simulation (50.000 runs in SAS/IML) is

$$p = 0 .002$$

such that the difference between the two variance components is highly significant. So, the test in this case decides for a smaller tube-to-tube dispersion among the new tubes.

It is striking that even if the construction principle for generalized fixed level tests was not designed for this situation of more than one model, it works in the same manner as before. The reason is, that the construction principle uses nothing more than independent χ^2 -variates, no matter from which model they come from.

Example 3

This example is taken from Gallo and Khuri (1990). The average daily gains (in pounds) of 65 steers from 9 sires and 3 ages of dam were reported in Damon and Harvey (1987, pp. 131,140). The data are given in table 3. The actual experiment was conducted at the U.S. Range Livestock Experiment Station in Miles City, Montana, over a 10-year period from 1947 through 1956 (see Shelby et al. (1963)). A total of 616 Hereford topcross steers were actually fed in this experiment.

Table 3: Average Daily Gain (in Punds) for 76 Steers

		Age				Age				Age	
Sire	3	4	5–up	Sire	3	4	5-up	Sire	3	4	5-up
1	2.24	2.41	2.58	4	2.50	2.44	2.54	7	2.57	2.64	2.37
	2.65	2.25	2.67		2.44	2.15	2.74		2.37		2.22
			2.71				2.50				1.90
			2.47				2.54				2.61
											2.13
											2.31
2	2.15	2.29	1.97	5	2.65	2.52	2.79	8	2.16	2.45	1.44
		2.26	2.14			2.67	2.33		3.33		1.72
			2.44				2.67		2.52		2.17
			2.52				2.69				
			1.72								
			2.75								
3	2.38	2.46	2.29	6	2.30	3.00	2.25	9	2.68	2.43	2.66
			2.30			2.49	2.49			2.36	2.46
			2.94				2.02			2.44	2.52
							2.31				2.42

For the data in Table 3 an unbalanced 2–way crossed classification model with mixed effects is used:

$$(6.10) y_{ijk} = \mu + \alpha_i + b_j + (\alpha b)_j + e_{ijk} ,$$

$$i = 1, \dots, r , j = 1, \dots, s , k = 1, \dots, \eta_{(i,j)} ,$$

$$\sum_{i=1}^r \alpha_i = 0 , b_j \sim (0, \sigma_b^2) , (\alpha b)_{ij} \sim (0, \sigma_{\alpha b}^2) , e_{ijk} \sim (0, \sigma_e^2) ,$$

$$b_i, (\alpha b)_{ij} \text{ and } e_{ijk} \text{ stochastically independent } .$$

Note, that the structure is the same as in Example 1, i.e. the model given in (6.1). The only difference is, that in (6.10) the first main effect is fixed while in (6.1) it is random. The following results show wide correspondence with the results from Example 1:

Especially we have

$$c=r\cdot s$$
 , $N=\sum n_{\omega}=65$, $\omega=(i,j)$, $\theta=(i,j,k)$, $q=2$, $m=4$,

and the basis transformation matrix Φ from (2.18) and matrix Λ , used for constructing the diagonalization matrix Q in formula (5.6), are given by

Using SAS/IML the following results are obtained (cf. section 3):

$$SS(e) = 2.267, \ \lambda_{max} = 1$$

 $SS_2(e) = 0.614, \ SS_b = 0.857, \ SS_{\alpha b} = 1.539.$

Then the generalized p-value for

(6.11)
$$H_0: \sigma_b^2 = \sigma_{\alpha b}^2 \quad \text{vs.} \quad H_1: \sigma_b^2 \neq \sigma_{\alpha b}^2$$

according to (4.8) can be computed as

(6.12)
$$p = 2 \cdot \min\{\Pr(T(Y, y, \sigma) > 1), \Pr(T(Y, y, \sigma) < 1)\}$$

with

(6.13)
$$T(Y,y,\sigma) = \frac{(r\sigma_b^2 + \sigma_{\alpha b}^2 + \lambda_{max}\sigma_e^2)\frac{ss_b}{SS_b} + r \cdot (\lambda_{max}\sigma_e^2)\frac{ss_2(e)}{SS_2(e)}}{r \cdot (\sigma_b^2 + \lambda_{max}\sigma_e^2)\frac{ss_{\alpha b}}{SS_{\alpha b}} + (\sigma_{\alpha b}^2 + \lambda_{max}\sigma_e^2)\frac{ss_{\alpha b}}{SS_{\alpha b}}}$$

and the result returned by 50.000 simulations is

$$p = 0 .34$$

such that the difference between the two variance components is not significant.

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