AN ABSTRACT OF THE THESIS OF

<u>Kathleen G. Purdy</u> for the degree of <u>Doctor of Philosophy</u> in <u>Statistics</u> presented on <u>May 8, 1998</u>. Title: <u>Confidence Intervals for Variance Components</u>.

Measuring the source and magnitude of components of variation has important applications in industrial, environmental and biological studies. This thesis considers the problem of constructing confidence intervals for variance components in Gaussian mixed linear models. A number of methods based on the usual ANOVA mean squares have been proposed for constructing confidence intervals for variance components in balanced mixed models. Some authors have suggested extending balanced model procedures to unbalanced models by replacing the ANOVA mean squares with mean squares from an unweighted means ANOVA. However, the unweighted means ANOVA is only defined for a few specific mixed models. In Chapter 2 we define a generalization of the unweighted means ANOVA for the three variance component mixed linear model and illustrate how the mean squares from this ANOVA may be used to construct confidence intervals for variance components. Computer simulations indicate that the proposed procedure gives intervals that are generally consistent with the stated confidence level, except in the case of extremely unbalanced designs. A set of statistics that can be used as an alternative to the generalized unweighted mean squares is developed in Chapter 3. The intervals constructed with these statistics have better coverage probability and are often narrower than the intervals constructed with the generalized unweighted mean squares.

Confidence Intervals for Variance Components

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Drs. Justus F. Seely and Youngjo Lee were involved in the development and editing of each manuscript.

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Confidence Intervals on Variance Components

Chapter 1

Introduction

Many statistical questions are concerned with identifying the source and magnitude of variation in data. Measuring this variability within a system has applications in environmental, industrial, and biological problems. To this end, researchers often require both point and interval estimates of the variance components that measure this variation. By modeling and estimating different components of variation researchers can determine which components are most important to their problem which will, in turn, help them improve the quality of industrial processes, identify important components of genetic variation, and improve the efficiency of sampling schemes.

This thesis discusses problems with multiple sources of variation when the random effects arise from a Gaussian process. Specifically, we consider confidence interval estimation for unbalanced mixed models with two or more components of variance. We choose to focus on confidence intervals rather than statistical tests since they are almost always more informative than simple statistical tests.

Many authors have considered the problem of constructing confidence intervals on variance components. Two of the earliest methods were proposed by Satterthwaite (1946) and Welch (1956). Although these methods were developed for balanced models, in practice they are often applied haphazardly to unbalanced models. Boardman (1974) and Wang (1990) reviewed several methods, including the Satterthwaite and Welch methods, for constructing confidence intervals on the among group variance component in the balanced random one-way model. Based on Monte Carlo simulations

they recommended three methods: the Tukey (1951)-Williams (1962), Moriguti (1954)-Bulmer (1957), and Howe (1974) methods. All of these methods are based on the usual ANOVA mean squares. Thomas and Hultquist (1976) described a technique to extend these methods to the unbalanced random one-way model. Based on simulations and analytical properties, they recommended replacing the usual ANOVA mean squares in the balanced model procedures with mean squares from an unweighted means ANOVA.

Ting, Burdick, Graybill, Jeyaratnam, and Lu (1990) proposed a method, referred to as the Modified Large Sample (MLS) method, for constructing confidence intervals on linear combinations of variance components for balanced mixed linear models with any number of variance components. The MLS method was extended to the unbalanced completely random nested model with any number of random effects and the unbalanced two-factor crossed model with or without interaction by Hernandez, Burdick and Birch (1992), Burdick and Graybill (1992), and Hernandez and Burdick (1993a, 1993b). Following the advice of Thomas and Hultquist, these authors recommended using unweighted mean squares, where an unweighted means ANOVA could be defined, in the MLS method to construct variance component confidence intervals for these models. However, as noted by Burdick and Graybill, intervals based on the unweighted mean squares can be very liberal for some unextremely unbalanced designs.

Eubank, Seely, and Lee (1998) generalized the unweighted means ANOVA to the two variance component mixed linear model by defining mean squares with properties similar to the unweighted mean squares. They recommended using these mean squares to construct confidence intervals on variance components in two variance component mixed linear models. This method appears to work well in many cases; however, for some extremely unbalanced designs these intervals can very liberal. An alternative interval was proposed by Lee, Seely, and Purdy (1998). Simulation studies indicate that this interval is generally consistent with the stated level and often narrower than intervals based on the generalized unweighted mean squares.

In Chapter 2 we extend the definition of the generalized unweighted mean squares, developed by Eubank et al., to the general three variance component mixed linear model. For balanced designs these generalized unweighted mean squares coincide with the usual ANOVA mean squares and they generally agree with the unweighted mean squares that have been previously defined for particular unbalanced designs. However, our definition is not restricted to classification models or designs with no missing cells. We illustrate how these generalized unweighted mean squares can be used to construct confidence intervals on linear combinations of variance components and give simulation results demonstrating that the proposed procedure produces intervals that are generally consistent with the stated confidence level, except for some extremely unbalanced designs. Additionally, we show how one could extend this generalization of the unweighted mean squares to models with more than three variance components.

The interval procedure proposed by Lee et al. is extended to the three variance component model in Chapter 3. Because intervals based on the unweighted mean squares can be liberal, this interval offers a good alternative to that approach. We present Monte Carlo simulations that compare the new interval to the MLS interval based on the unweighted mean squares for various designs. These simulations show that the new interval not only has better coverage probability but is also generally narrower than the interval constructed with unweighted mean squares.

Generalizing Unweighted Mean Squares for the General Mixed Linear Model

Kathleen G. Purdy, Justus F. Seely, and Youngjo Lee

2.1 Abstract

As summarized in Burdick and Graybill (1992), a number of ANOVA-type procedures are available for constructing confidence intervals on linear combinations of variance components for particular mixed linear models. The procedures for balanced designs are based on the usual ANOVA mean squares and some authors have suggested extending these procedures to unbalanced designs by replacing the usual ANOVA mean squares with mean squares from an unweighted means ANOVA. However, this technique of replacement is restricted to models and designs where the unweighted mean squares are defined. Eubank, Seely, and Lee (1998) removed this restriction for the two variance component mixed linear models and in this paper we extend their results to three variance component mixed linear models. For balanced designs, the mean squares from this new ANOVA coincide with the usual ANOVA mean squares and they generally agree with the unweighted mean squares that have been defined for particular unbalanced designs. We illustrate how the mean squares from this new ANOVA may be used to construct confidence intervals on linear combinations of variance components. Computer simulations indicate that the proposed procedure produces intervals that are generally consistent with the stated confidence level.

2.2 Introduction

In many biological and industrial applications, researchers require confidence intervals on functions of variance components. A number of methods have been developed for constructing confidence intervals on linear combinations of variance components in balanced models and some of these methods have been extended to particular unbalanced models. In this paper we propose a technique to construct confidence intervals for variance components in a very general three variance component mixed linear model. This technique for constructing intervals can be easily extended to models with more than three variance components.

As an illustration, consider the blood pH data presented in Box 10.4 of Sokal and Rohlf (1981). In the experiment 15 dams (female mice) were mated with either two or three sires. Each sire was mated to a different dam giving a total of 37 sires. The response variable is the blood pH of a female offspring from a given dam-sire pair. Sokal and Rohlf suggested the following random-effects model to analyze these data

(2.1) $y_{ijm} = \mu + a_i + b_{ij} + e_{ijm}$

 $(i = 1, ..., 15, j = 1, ..., J_i$, and $m = 1, ..., M_{ij}$) where μ is an unknown constant and a_i , the dam effect, b_{ij} , the sire effect, and e_{ijm} are mutually independent normal random variables with zero means and variances σ_a^2 , σ_b^2 , and σ^2 , respectively. A researcher may be interested in determining the variation due to the dam effect or the variation due to both the dam and sire effects. These questions of interest can be answered by constructing confidence intervals on the variance component σ_a^2 or the sum $\sigma_a^2 + \sigma_b^2$, respectively.

A review of the existing methods for constructing variance component confidence interval in three variance component mixed linear models is given in the next section. In Section 2.4 we develop a generalization of the unweighted mean squares for the three variance component mixed linear model and demonstrate how these mean squares can be used to construct confidence intervals. Section 2.5 gives properties that uniquely define the new mean squares. Simulation results are given in Section 2.6 and in Section 2.7 we give a SAS[®] routine that may be used to generate the generalized unweighted mean squares. Extensions to models with more than three variance components are given in Section 2.8. Concluding remarks are given in Section 2.9.

Throughout this paper we will use the notation A^+ , C(A), and $C(A)^{\perp}$ to denote the Moore-Penrose inverse of a matrix A, the column space of A, and its orthogonal

complement, respectively. We will also use the notation P_A to denote the orthogonal projection operator on the column space of A; that is, $P_A = A(A'A)^+A'$.

2.3 Review of Existing Methods

Let Y be an n-dimensional multivariate normal (MVN_n) random vector with mean and covariance matrix

(3.1)
$$E(Y) = X\beta \text{ and } Cov(Y) = \sigma_a^2 V_A + \sigma_b^2 V_B + \sigma^2 I$$

where β , $\sigma^2 > 0$, σ_a^2 , $\sigma_b^2 \ge 0$ are unknown parameters, X, V_A, V_B are known matrices such that V_A and V_B are nonnegative definite (n.n.d.), and $r = n - rank(X, V_A, V_B)$ is positive. Let $s_a = rank(X, V_A, V_B) - rank(X, V_B)$, $s_b = rank(X, V_A, V_B) - rank(X, V_A)$, $t_a = rank(X, V_A) - rank(X)$, and $t_b = rank(X, V_B) - rank(X)$.

Consider the problem of constructing a confidence interval on the parameter

(3.2)
$$\gamma = k_a \sigma_a^2 + k_b \sigma_b^2 + k \sigma^2$$

where k_a , k_b , and k are known constants. Suppose $\hat{\gamma} = c_1S_1 + c_2S_2 + c_3S_3$ where S_1 , S_2 , and S_3 are statistics and c_1 , c_2 , c_3 are constants such that

(3.3) (a) $\hat{\gamma}$ is unbiased for γ ;

- (b) $q_i S_i / E(S_i) \sim \chi^2(q_i)$ for i = 1,2,3, where q_1, q_2, q_3 are known integers;
- (c) S_1 , S_2 , and S_3 are mutually independent.

For example, consider model (2.1) and suppose $J_i = J$ and $M_{ij} = M$ for all *i*, *j*. Let MSA, MSB, and MSE be the usual ANOVA mean squares for the dam effect, the sire effect, and the error, respectively. It is well known that $S_1 = MSA$ with $q_1 = 14$, $S_2 = MSB$ with $q_2 = 15(J - 1)$, and $S_3 = MSE$ with $q_3 = 15J(M - 1)$ satisfy (b) and (c). Thus, for given k_a , k_b , and k, one may select c_1 , c_2 , and c_3 so that (3.3) is satisfied.

Methods for constructing confidence intervals on γ under assumptions (3.3) have been proposed by Satterthwaite (1946), Welch (1956), Graybill and Wang (1980), and Ting, Burdick, Graybill, Jeyaratnam, and Lu (1990). These methods *generally* produce approximate intervals. The word *generally* is used here because the methods are exact for special cases. Monte Carlo simulations performed by Graybill and Wang and Ting et al. indicate that of these four methods the Graybill-Wang method and the Ting et al. method can be recommended. In particular, the simulations indicated that the Graybill-Wang interval is generally consistent with the stated confidence level when γ and all of the c_i coefficients are nonnegative but that this interval procedure cannot be recommended otherwise. The method proposed by Ting et al., however, performs well for any choice of the c_i with no restriction on the sign of γ .

The Graybill-Wang two-sided $1 - 2\alpha$ confidence interval for γ based on assumptions (3.3) is

(3.4)
$$\left[\widehat{\gamma} - \sqrt{\sum_{i=1}^{3} G_i^2 c_i^2 S_i^2}; \quad \widehat{\gamma} + \sqrt{\sum_{i=1}^{3} H_i^2 c_i^2 S_i^2}\right],$$

and the two-sided $1 - 2\alpha$ confidence interval on γ proposed by Ting et al. under assumptions (3.3) is

(3.5)
$$\left[\widehat{\gamma} - \sqrt{V_{\rm L}} \; ; \; \widehat{\gamma} + \sqrt{V_{\rm U}} \; \right],$$

where

$$\begin{split} \mathbf{V}_{\mathrm{L}} &= \sum_{\substack{i=1\\c_i>0}}^{3} \mathbf{G}_i^2 \mathbf{c}_i^2 \mathbf{S}_i^2 + \sum_{\substack{j=1\\c_j<0}}^{3} \mathbf{H}_j^2 \mathbf{c}_j^2 \mathbf{S}_j^2 + \sum_{\substack{i=1\\c_i>0}}^{3} \sum_{\substack{j=1\\c_i>0}}^{3} \mathbf{G}_{ij} \mathbf{c}_i |\mathbf{c}_j| \mathbf{S}_i \mathbf{S}_j + \sum_{\substack{i=1\\c_i>0}}^{2} \sum_{\substack{j>i\\c_j>0}}^{3} \mathbf{G}_{ij}^* \mathbf{c}_i \mathbf{c}_j \mathbf{S}_i \mathbf{S}_j \,, \\ \mathbf{V}_{\mathrm{U}} &= \sum_{\substack{i=1\\c_i>0}}^{3} \mathbf{H}_i^2 \mathbf{c}_i^2 \mathbf{S}_i^2 + \sum_{\substack{j=1\\c_j<0}}^{3} \mathbf{G}_j^2 \mathbf{c}_j^2 \mathbf{S}_j^2 + \sum_{\substack{i=1\\c_i>0}}^{3} \sum_{\substack{j=1\\c_i>0}}^{3} \mathbf{H}_i \mathbf{c}_i |\mathbf{c}_j| \mathbf{S}_i \mathbf{S}_j + \sum_{\substack{i=1\\c_i<0}}^{2} \sum_{\substack{j>i\\c_j<0}}^{3} \mathbf{H}_{ij}^* \mathbf{c}_i \mathbf{c}_j \mathbf{S}_i \mathbf{S}_j \,, \end{split}$$

$$G_i = 1 - \frac{1}{F_{\alpha:q_i,\infty}}$$
, and $H_i = \frac{1}{F_{1-\alpha:q_i,\infty}} - 1$,
 $(F_{\alpha:q_i,q_i} = 1)^2 - G_i^2 F_{\alpha:q_i,q_i,q_i}^2 - H_i^2$ $(1 - F_{1-\alpha:q_i,\infty})$

$$G_{ij} = \frac{(F_{\alpha:q_i,q_j} - 1)^2 - G_i^2 F_{\alpha:q_i,q_j}^2 - H_j^2}{F_{\alpha:q_i,q_j}}, \qquad H_{ij} = \frac{(1 - F_{1-\alpha:q_i,q_j})^2 - H_i^2 F_{1-\alpha:q_i,q_j}^2 - G_j^2}{F_{1-\alpha:q_i,q_j}},$$

$$\mathbf{G}_{ij}^* = \left\lfloor \left(1 - \frac{1}{\mathbf{F}_{\alpha:\mathbf{q}_i + \mathbf{q}_j,\infty}} \right)^2 \frac{(\mathbf{q}_i + \mathbf{q}_j)^2}{\mathbf{q}_i \mathbf{q}_j} - \frac{\mathbf{q}_i \mathbf{G}_i^2}{\mathbf{q}_j} - \frac{\mathbf{q}_j \mathbf{G}_j}{\mathbf{q}_i} \right\rfloor,$$

$$\mathbf{H}_{ij}^* = \left[\left(1 - \frac{1}{\mathbf{F}_{\alpha:\mathbf{q}_i + \mathbf{q}_j,\infty}} \right)^2 \frac{(\mathbf{q}_i + \mathbf{q}_j)^2}{\mathbf{q}_i \mathbf{q}_j} - \frac{\mathbf{q}_i \mathbf{G}_i^2}{\mathbf{q}_j} - \frac{\mathbf{q}_j \mathbf{G}_j^2}{\mathbf{q}_i} \right],$$

and $F_{x:n,m}$ represents the upper x percentage point of the F distribution with n and m degrees of freedom. If it is known that $\gamma \ge 0$ then any negative bounds in (3.4) or (3.5) are defined to be zero. Note that procedures (3.4) and (3.5) are often referred to in the literature as Modified Large Sample (MLS) procedures.

If model (3.1) is unbalanced, then in most cases there does not exist a partitioning of the error space sum of squares, i.e., the sum of squares of the least squares residuals, that leads to three independent chi-squared random variables. That is, for most unbalanced designs based on model (3.1) we cannot find statistics S_1 , S_2 , and S_3 that use all of the data and satisfy conditions (3.3b) and (3.3c). To circumvent this difficulty, Thomas and Hultquist (1978) suggested a technique to extend methods based on exact distributional assumptions to the unbalanced random one-way model. They recommended replacing the ANOVA mean squares in a balanced model procedure with statistics that are independent and distributed approximately chi-squared. Based on simulation results and analytical properties, Thomas and Hultquist recommended using mean squares from an unweighted means ANOVA. Hernandez and Burdick (1993a, 1993b) and Hernandez, Burdick and Birch (1992) investigated using the Thomas-Hultquist technique (i.e., replacing ANOVA mean squares with mean squares from an unweighted means ANOVA) for two classification models. They considered the completely random nested model with three variance components and the random twoway additive model with interaction and no missing cells and, based on simulation results, recommended using the unweighted mean squares to construct confidence intervals on variance components for these models. The Thomas-Hultquist idea has been extended to other models where an unweighted means ANOVA is defined, as summarized in Burdick and Graybill (1992). A limitation of this technique of replacement is that it can only be used for models and designs where an unweighted

means ANOVA can be constructed. Eubank, Seely, and Lee (1998) showed how to remove this limitation in a general two variance component model by defining mean squares with properties similar to the unweighted mean squares. Unlike the definition of a unweighted means ANOVA, their definition does not require that all cell sample sizes are positive and may be used with covariates or continuous type design variables. Similar to previous authors, Eubank et al. recommended using these generalized unweighted mean squares in the MLS procedures to construct confidence intervals on variance components. In this paper we extend the Eubank et al. results. In particular, we define a generalization of the unweighted means ANOVA for the general three variance component mixed linear model and describe how this generalization can be extended to models with more than three variance components. For balanced designs the mean squares from this ANOVA coincide with the usual ANOVA mean squares and they generally agree with the unweighted mean squares that have been previously defined for particular unbalanced designs. (See Eubank et al. for an example of where these mean squares disagree). Our simulation results indicate that intervals constructed with these generalized unweighted mean squares are generally consistent with the stated confidence level.

2.4 Development of the Generalized Unweighted Mean Squares

In Section 2.4.1 we define the generalized unweighted mean squares for a completely nested model. These mean squares are developed so that they share properties of the unweighted mean squares in the completely random nested classification model considered by Hernandez, Burdick, and Birch (1992). Then in Section 2.4.2 we extend the definition to the general model (3.1) by transforming the data vector such that the resulting model is either a nested model, in which case the procedure in Section 2.4.1 can be employed to define the generalized unweighted mean

squares, or a two variance component model, in which case the definition given in Eubank et al. (1998) is applicable.

2.4.1 The Completely Nested Model

Consider model (3.1) and suppose that

$$(4.1) C(X) \subset C(V_A) \subset C(V_B).$$

Assume that s_b and t_a are both positive. Let A and B be any matrices of dimensions $n \times a$ and $n \times b$, respectively, such that $V_A = AA'$ and $V_B = BB'$ where $a = rank(V_A)$ and $b = rank(V_B)$. Note that under condition (4.1), r = n - b, $s_b = b - a$, and $t_a = a - rank(X)$.

In this section we define statistics MSA, MSB, and MSE for model (3.1) under condition (4.1) with properties similar to unweighted mean squares and demonstrate how these statistics can be used to construct a confidence interval for γ in (3.2).

First consider the error mean square, say MSE. In the nested classification model of Hernandez et al. (1992), the MSE has the property that $MSE/\sigma^2 \sim \chi^2(k)/k$ for some k. If we suppose that the MSE for model (3.1) has the chi-squared property with k as large as possible, then Proposition 3.3 in Seely and El-Bassiouni (1983), implies that $k \leq r$ and that there exists only one quadratic form with k = r. For model (3.1), this unique quadratic form may be expressed as

$$MSE = Y'NY/r,$$

where N is the orthogonal projection operator on the space orthogonal to the columns of X, A, and B, i.e., $N = I - P_{(X,A,B)}$.

Now let us turn to the mean square for B, say MSB. For the nested classification model of Hernandez et al., MSB is based on the cell means and has the property that $MSB/\sigma_b^2 \sim \chi^2(k)/k$ when $\sigma^2 = 0$. In the nested classification model the cell means are L'Y where $L = B(B'B)^{-1}$. Thus, imitating this procedure for the general nested model,

we base MSB on U = L'Y. Note that U ~ MVN_b with E(U) = L'X β and Cov(U) = $\sigma_a^2 \widetilde{A} \widetilde{A}' + \sigma_b^2 I + \sigma^2 D$ where $\widetilde{A} = L'A$ and D = L'L. Hence, if $\sigma^2 = 0$ then using Proposition 3.3 in Seely and El-Bassiouni there exists, as above, a unique quadratic form in U, MSB, such that MSB/ $\sigma_b^2 \sim \chi^2(k)/k$ where $k = b - \operatorname{rank}(L'X, \widetilde{A}) = s_b$. For model (4.1), this quadratic form may be expressed as (4.3) MSB = U'N_BU/s_b ,

where N_B is the orthogonal projection operator on the space orthogonal to the columns of L'X and \widetilde{A} . Note that $\mathcal{C}(L'X)\subset\mathcal{C}(\widetilde{A})$; hence, $N_B=I-P_{\widetilde{A}}.$

The mean square for A, say MSA, in the nested classification model of Hernandez et al. is based on the means of the cell means and has the property that $MSA/\sigma_a^2 \sim \chi^2(k)/k$ when $\sigma^2 = \sigma_b^2 = 0$. In the nested classification model the means of the cell means are T = K'U where $K = \widetilde{A} (\widetilde{A}'\widetilde{A})^{-1}$. Again we imitate this procedure and base MSA on T. Note that $T \sim MVN_a$ with $E(T) = X^*\beta$ where $X^* = K'L'X$ and $Cov(T) = \sigma_a^2 I + \sigma_b^2 K'K + \sigma^2 K'DK$. Thus, if $\sigma^2 = \sigma_b^2 = 0$ then there is a unique quadratic form in T, MSA, such that $MSA/\sigma_a^2 \sim \chi^2(k)/k$ where $k = a - rank(X^*) = t_a$. For model (4.1), this quadratic form may be expressed as

(4.4)
$$MSA = T'N_AT/t_a ,$$

where N_A is the is the orthogonal projection operator on the space orthogonal to the columns of X^* , i.e., $N_A = I - P_{X^*}$.

We have now described three mean squares MSA, MSB, and MSE that are defined for the completely nested model with three variance components. These mean squares are a generalization of the unweighted mean squares defined in Hernandez et al. (1992). However, mean squares (4.2)-(4.4) are not restricted to classification models as is the definition of the unweighted mean squares given in Hernandez et al. For example, covariates can be accommodated by definitions (4.2)-(4.4). Next we illustrate how these mean squares can be used to construct confidence intervals for γ in (3.2). Let

(4.5)
$$W = trace(N_BD)/s_b$$

and

(4.6)
$$v_b = trace(N_A K' K)/t_a$$
 and $v = trace(N_A K' D K)/t_a$

Then E(MSE) = σ^2 , E(MSB) = $\sigma_b^2 + w\sigma^2$, and E(MSA) = $\sigma_a^2 + v_b\sigma_b^2 + v\sigma^2$. An

unbiased estimator of γ based on MSE, MSB, and MSA is given by

(4.7)
$$\widehat{\gamma} = c_1 MSA + c_2 MSB + c_3 MSE$$

where

(4.8)
$$c_1 = k_a, c_2 = k_b - k_a v_b, and c_3 = w(k_a v_b - k_b) - k_a v + k_b$$

Hence, one can construct a confidence interval for γ by replacing S₁, S₂, S₃, q₁, q₂, and q₃ in either (3.4) or (3.5), whichever is appropriate, with MSA, MSB, MSE, t_a, s_b, and r, respectively.

Example 2.4.9. Consider the blood pH data given in Box 10.4 of Sokal and Rohlf (1981) and the suggested model given by (2.1). We can express model (2.1) in matrix form as

$$Y = 1\mu + Aa + Bb + e.$$

Then

$$E(Y) = 1\mu$$
 and $Cov(Y) = \sigma_a^2 V_A + \sigma_b^2 V_B + \sigma^2 I_A$

where $V_A = AA'$ and $V_B = BB'$. There are 160 offspring, 15 dams, and 37 sires in the study; hence, r = 123, $s_b = 22$, and $t_a = 14$. Using definitions (4.2)-(4.6), we obtain MSE = 24.74, MSB = 8.68, MSA = 12.97, w = 0.237, v_b = 0.422, and v = 0.101. An approximate two-sided confidence interval on $\gamma = \sigma_a^2$ can be obtained by replacing S₁, S₂, S₃, q₁, q₂, and q₃ with MSA, MSB, MSE, t_a, s_b, and r, respectively, and setting $c_1 = 1$, $c_2 = -0.422$, and $c_3 = -0.001$ in interval (3.5). This procedure yields the approximate 95% confidence interval [2.30; 28.5]. Similarly, setting $c_1 = 1$,

 $c_2 = 0.578$, and $c_3 = 0.762$, an unbiased estimate of $\gamma = \sigma_a^2 + \sigma_b^2 + \sigma^2$ is $\hat{\gamma} = 36.84$ and an approximate 95% confidence interval on γ using (3.4) is [29.4; 57.6]. \Box

It is important to note that for model (2.1) the means squares (4.3) and (4.4) are not defined exactly as in Hernandez et al. (1992). The resulting estimators and confidence limits, however, are identical. The unweighted mean squares in Hernandez et al. are scaled so that the coefficient of the random error variance component σ^2 in the expected mean squares is one, while mean squares (4.3) and (4.4) are scaled so that the coefficient of σ_b^2 in E(MSB) is one and the coefficient of σ_a^2 in E(MSA) is one.

2.4.2 The General Model

Consider the general three variance component model (3.1) and let m = n - rank(X). In this section we define mean squares MSE, MSB, and MSA for the general model that have properties similar to the mean squares in an unweighted means ANOVA. In particular, in defining MSE, MSB, and MSA we will incorporate two general properties of the unweighted mean squares. The first property, which is described more fully below, is that the mean squares are translation invariant. The second property that we incorporate is that the distribution of the mean squares be dependent upon as few parameters as possible. For example, this means that the distribution of MSB should depend on σ_b^2 and as few other parameters as possible. Goodnight (1976) refers to quadratic estimators with these two properties as maximally invariant quadratic estimators.

The property of translation invariance is equivalent to reducing to the least squares residuals, that is, transforming Y so that the resulting model has mean zero. To this end, let Q be any matrix such that $C(Q) = C(X)^{\perp}$ and Q'Q = I, and let Z = Q'Y. Then Z is a one-to-one linear transformation of the least squares residuals. Furthermore, $Z \sim MVN_m$ with zero mean and covariance matrix

(4.10)
$$\operatorname{Cov}(Z) = \sigma_{a}^{2} W_{A} + \sigma_{b}^{2} W_{B} + \sigma^{2} I$$

where $W_A = Q'V_AQ$ and $W_B = Q'V_BQ$. Note that the distribution of Z does not depend on the parameter β so that trying to get a quadratic forms in Z that depend on as few parameters as possible we need only be concerned with the variance component parameters σ^2 , σ_b^2 , and σ_a^2 .

To obtain the error mean square MSE for model (3.1) we use the procedure from Section 2.4.1. That is, the MSE is defined so that $MSE/\sigma^2 \sim \chi^2(r)/r$. Again, using the Seely-El-Bassiouni result, there exists only one quadratic form with this property, in particular, $MSE = Z'(I - P_{(W_A, W_B)})Z/r = Y'(I - P_{(X, V_A, V_B)})Y/r$. Note that the distribution of MSE depends only on σ^2 so that it has the property that its distribution depends on as few parameters as possible.

Next consider the mean square for the effect corresponding σ_a^2 , namely MSA. Now we want the distribution of MSA to depend on σ_a^2 , but as few other parameters as possible. First note that it is impossible to define a quadratic form in Z whose distribution depends on σ_a^2 but not on σ^2 . So the only other parameter that we need to be concerned with is σ_b^2 . Suppose that $s_a > 0$. Let U = K'Z where K is any matrix such that $C(K) = C(W_A, W_B) \cap C(W_B)^{\perp}$. Then E(U) = 0 and $Cov(U) = \sigma_a^2 K' W_A K + \sigma^2 K' K$. Thus, when $s_a > 0$ we can define a quadratic form in U whose distribution does not depend on σ_b^2 . Furthermore, since U is a two variance component model, we can employ the method described in Eubank et al. to obtain MSA. This gives

$$MSA = U'(K'W_AK)^+U/s_a.$$

Note that the resulting mean square has the property $MSA/\sigma_a^2 \sim \chi^2(s_a)/s_a$ when $\sigma^2 = 0$.

Now suppose $s_a = 0$, $s_b > 0$, and $t_a > 0$ then model (4.10) is completely nested and, hence, we can apply the procedure described in the previous section to the transformed data vector Z to obtain MSA for the general model (3.1). Let G and H be any full column rank matrices such that $GG' = W_A$ and $HH' = W_B$. Then

 $MSA = Z'TT'Z/t_a ,$

where $T = H(H'H)^{-1}\widetilde{G} (\widetilde{G}'\widetilde{G})^{-1}$ and $\widetilde{G} = (H'H)^{-1}H'G$. Notice that the resulting mean square has the property $MSA/\sigma_a^2 \sim \chi^2(t_a)/t_a$ when $\sigma^2 = \sigma_b^2 = 0$. Finally, if both s_a and t_a are zero then MSA is undefined.

To obtain, MSB, the mean square for the effect corresponding to σ_b^2 , we simply interchange the roles of V_A and V_B in this section and follow the procedure used to obtain MSA. That is, one examines whether s_b is positive or s_b = 0, s_a > 0, and t_b > 0. A confidence interval for $\gamma = k_a \sigma_a^2 + k_b \sigma_b^2 + k \sigma^2$ based on MSE, MSB, and MSA and their associated degrees of freedom can then be constructed as described in Section 2.4.1.

Example 2.4.13. Harville and Fenech (1985) presented some data consisting of the weights at birth of 62 single-birth male lambs in Table 1 of their paper. The lambs represented in these data came from five distinct population lines. Each lamb was the offspring of one of 23 rams, and each lamb had a different dam. The age of the dam was recorded for each lamb. A possible model for these data is the mixed linear model

$$\mathbf{y}_{ijkd} = \boldsymbol{\mu} + \delta_i + \pi_j + \mathbf{a}_{jk} + \mathbf{b}_{ijk} + \mathbf{e}_{ijkd}$$

 $(i = 1, 2, 3, j = 1, ..., 5, k = 1, ..., m_j$, and $d = 1, ..., n_{ijk}$) where δ_i , the age effect, and π_j , the line effect, are fixed, and a_{jk} , the random sire (within line) effect, b_{ijk} , the interaction of sire and age, and e_{ijkd} are normal and independent with zero means and variances σ_a^2 , σ_b^2 , and σ^2 , respectively. This model can be expressed in matrix form as

$$Y = X\beta + Aa + Bb + e$$

where X includes all fixed effects. Then $E(Y) = X\beta$ and $Cov(Y) = \sigma_a^2 V_A + \sigma_b^2 V_B + \sigma^2 I$ where $V_A = AA'$ and $V_B = BB'$. The mean squares are MSE = 2.36, MSB = 2.56, and MSA = 3.03 with degrees of freedom r = 24, $s_b = 13$, and $t_a = 18$, respectively. An approximate two-sided confidence interval on $\gamma = \sigma_a^2$ can be constructed by replacing S₁, S₂, S₃, q₁, q₂, and q₃ with MSA, MSB, MSE, t_a, s_b, and r, respectively, and setting c₁ = 1, c₂ = -0.756, and c₃ = -0.058 in (3.5). The resulting 95% confidence interval is [0; 4.65]. \Box

2.5 Properties of the Mean Squares

Consider the general mixed linear model (3.1). Recall that $r = n - rank(X, V_A, V_B)$, $s_a = rank(X, V_A, V_B) - rank(X, V_B)$, $s_b = rank(X, V_A, V_B) - rank(X, V_A)$, and $t_a = rank(X, V_A) - rank(X)$. The following propositions uniquely characterize mean squares MSE and MSA defined in Section 2.4.2. Note that in each proposition the distribution statements refer to model (3.1).

Proposition 2.5.1. Suppose r > 0 and Q is a symmetric matrix such that for all β , σ_a^2, σ_b^2 , and $\sigma^2, Y'QY/\sigma^2 \sim \chi^2(r)$. Then Y'QY = rMSE.

See Seely and El-Bassiouni (1983) for a proof of Proposition 2.5.1.

Proposition 2.5.2. Assume $s_a > 0$ and suppose M is a symmetric matrix such that (a) $Y'MY/\sigma_a^2 \sim \chi^2(s_a)$ for all β , σ_b^2 , $\sigma_a^2 > 0$, and $\sigma^2 = 0$;

(b) Cov(MY, $(I - P_{(X,V_A,V_B)})Y) = 0$ for all β , σ_a^2 , σ_b^2 , and σ^2 .

Then M is unique and $Y'MY = s_aMSA$ in (4.11).

Note that part (b) ensures that MSA and MSE are independent. A proof of this proposition is given in Section 2.10.

Proposition 2.5.3. Assume $s_a = 0$, $s_b > 0$, and $t_a > 0$. Suppose M is a nonnegative definite matrix such that

- (a) $Y'MY/\sigma_a^2 \sim \chi^2(t_a)$ for all β , $\sigma_a^2 > 0$, and $\sigma^2 = \sigma_b^2 = 0$;
- (b) Cov(MY, $(I P_{(X,V_A,V_B)})Y) = 0$ for all β , σ_a^2 , σ_b^2 , and σ^2 ;
- (c) $\operatorname{Cov}(\operatorname{MY}, (\operatorname{P}_{(X,V_A,V_B)} \operatorname{P}_{(X,V_A)})Y) = 0$ for all β , σ_a^2 , σ_b^2 , and $\sigma^2 = 0$.

Then M is unique and $Y'MY = t_aMSA$ in (4.12).

A proof of Proposition 2.5.3 is given in Section 2.10. Note that the assumption $s_a = 0$ implies that $C(V_A) \subset C(X, V_B)$. Also note that part (b) of this proposition ensures that MSA is independent of MSE and part (c) implies that MSA and MSB are independent when $\sigma^2 = 0$.

Using the above propositions, we can obtain alternative expressions for MSA. First consider the case when $s_a > 0$. Let L be any matrix such that $C(L) = C(X, V_A, V_B) \cap C(X, V_B)^{\perp}$ and set

$$M_1 = L(L'V_AL)^+L'.$$

It can be shown that M_1 is symmetric and M_1 substituted for M in Proposition 2.5.2 satisfies (a) and (b). Hence, $Y'M_1Y/s_a = MSA$ in (4.11) giving us an alternative expression for MSA when $s_a > 0$.

Next assume $s_a = 0$, $s_b > 0$, and $t_a > 0$. Let K be any matrix such that $C(K) = C(X, V_BN, V_B) \cap C(X, V_BN)^{\perp}$ and $N = I - P_{(X,V_A)}$. Set $M_2 = K(K'V_AK)^+K'$.

One can show that M₂ is n.n.d. and that M₂ substituted for M in Proposition 2.5.3 satisfies (a)-(c). Hence, $Y'M_2Y/t_a = MSA$ in (4.12).

Note also that the mean squares MSA and MSE defined in Section 2.4.1 for the completely nested model (4.1) are equivalent to MSA and MSE defined for the general model (3.1) when $C(X) \subset C(V_A) \subset C(V_B)$. That is, if $C(X) \subset C(V_A) \subset C(V_B)$ then, for example, MSA (4.4) is equivalent to MSA (4.12). Additionally, by interchanging V_A and V_B in this section, uniqueness propositions, similar to Propositions 2.5.2 and 2.5.3, as well as alternative expressions may be given for mean square MSB.

2.6 Simulation Results

In this section we give simulation results for the interval proposed in Section 2.4 for two models based on (3.1). We obtained simulation results for additional models,

however, the examples given below illustrate the general properties and/or potential problems with this method. The performance of the confidence interval procedure is measured by the coverage probability. All of the reported intervals are two-sided 95% confidence intervals with equal tail probability. We also considered 99% confidence intervals and found that the performance of these intervals was similar to the 95% confidence intervals, and hence, the results are not reported. Different values of the ratios $\rho_a = \sigma_a^2/(\sigma_a^2 + \sigma_b^2 + \sigma^2)$ and $\rho_b = \sigma_b^2/(\sigma_b^2 + \sigma^2)$ are considered for each design. Each simulation result is based on 2000 pseudo-random data sets generated in S-PLUS. This results in a standard error of approximately 0.5% on the coverage probabilities given in the tables below.

Example 2.6.1. Consider the following two-way additive model with interaction (6.2) $Y_{ijk} = \mu + \tau_i + a_j + b_{ij} + e_{ijk}$

 $(i = 1, ..., I, j = 1, ..., J, k = 1, ..., n_{ij})$ where μ and τ_i are fixed effects and a_j , b_{ij} , and e_{ijk} are mutually independent normal random variables with zero means and variances σ_a^2 , σ_b^2 , and σ^2 , respectively. Consider placing a confidence interval on σ_a^2 . When all of the $n_{ij} > 0$ the interval proposed in Section 2.4 is identical to the interval recommended by Hernandez and Burdick (1993a). Hernandez and Burdick considered several unbalanced designs where all $n_{ij} > 0$ and found that the proposed interval generally maintained the stated confidence level for the designs considered. The Hernandez-Burdick unweighted mean squares, however, cannot be defined when some $n_{ij} = 0$; whereas the definition of the generalized unweighted mean squares given in Section 2.3 does allow for missing cells. For example, consider a design where I = 3, J = 4, $n_{11} = n_{12} = n_{21} = n_{24} = n_{32} = n_{34} = 10$, $n_{13} = n_{33} = 1$, and $n_{14} = n_{22} = n_{23} = n_{31} = 0$. The degrees of freedom corresponding to the generalized unweighted mean squares MSA, MSB, and MSE are $t_a = 3$, $s_b = 2$, and r = 54, respectively. Note that for model (6.2), $s_a = 0$. The simulation results for confidence intervals on σ_a^2 for this design are given in Table 2.1.

We considered several designs of model (6.2), that is, different values of I and J and different n_{ij} patterns, with and without missing cells and found that the proposed interval on σ_a^2 generally maintains the stated confidence level. We did find, however, that for some types of extremely unbalanced designs, the proposed method can produce liberal intervals for small values of ρ_a . A prototype of such a design is given in the next example. In addition to confidence intervals on σ_a^2 , we considered intervals on $\sigma_a^2 + \sigma_b^2 + \sigma^2$ and obtained similar results. \Box

Table 2.1Confidence coefficients for intervals on σ_a^2 in Example 2.6.1 with stated level of 95%

				$ ho_{ m a}$		
		0.01	0.25	0.50	0.75	0.99
	0.01	94.6	95.0	95.0	95.6	94.0
$ ho_{ m b}$	0.50	94.9	94.9	96.5	96.5	94.5
	0.99	93.4	95.6	95.7	96.5	94.5

Example 2.6.3. Consider the following mixed model with $n = \sum_{ij} n_{ij}$ observations and a single covariate

(6.4)
$$Y_{ijk} = \beta_0 + \beta_1 x_i + \mathbf{a}_i + \mathbf{b}_{ij} + \mathbf{e}_{ijk}$$

 $(i = 1, ..., I, j = 1, ..., m_i, k = 1, ..., n_{ij})$ where β_0 and β_1 are fixed effects, the x_i are known constants and a_i , b_{ij} and e_{ijk} are mutually independent normal random variables with zero means and variances σ_a^2 , σ_b^2 , and σ^2 , respectively. Let x be the n × 1

vector composed of the x_i s. Consider a design with I = 6, $m_i = 2$, for i = 1, ..., 5, $m_6 = 50$, $n_{ij} = 2$ for all i, j, and the following covariate vector:

$$\mathbf{x}' = (1, 1, 2, 2, 3, 3, -1, -1, -2, -2, -3, -3, \dots, -3)$$

Then the degrees of freedom associated with the generalized unweighted mean squares MSA, MSB, and MSE are $t_a = 4$, $s_b = 24$, and r = 30, respectively. Note that for model (6.4), $s_a = 0$. Monte Carlo simulations of confidence intervals on σ_a^2 yielded minimum and maximum coverage probabilities of 94.2 and 95.6, respectively. Hence, for this design the coverage probabilities are very close to the stated level.

Now consider a design with I = 6, $m_i = 12$, for i = 1, ..., 5, $m_6 = 2$, and $n_{ij} = 2$ for all *i*, *j* and with the same covariate values for x_i , i = 1, ..., 6, as in the previous design. The degrees of freedom associated with the generalized unweighted mean squares MSA, MSB, and MSE for this design are $t_a = 4$, $s_b = 25$, and r = 31, respectively. The simulation results, presented in Table 2.2, indicate that for this design the proposed method produces intervals with confidence levels close to the stated level except when $\rho_a = 0.01$. We considered other designs with this type of pattern and obtained similar results; that is, the intervals tended to be liberal for small values of ρ_a for this type of unbalanced design. \Box

Table 2.2 Confidence coefficients for intervals on σ_a^2 in Example 2.6.3 with stated level of 95%

		$ ho_{ m a}$					
		0.01	0.25	0.50	0.75	0.99	
	0.01	92.0	94.1	95.1	95.4	94.4	
$ ho_{ m b}$	0.50	91.9	94.2	95.7	94.4	94.6	
	0.99	91.9	94.7	94.3	94.6	95.4	

2.7 Calculating the Mean Squares in SAS®

Consider model (3.1) and assume $s_a = 0$, $s_b > 0$, and $t_a > 0$. Let A and B be any matrices such that $V_A = AA'$ and $V_B = BB'$. The following SAS[®] code can be used to generate the mean squares MSE, MSB, and MSA defined in Section 2.4.2. This code can be easily modified to compute MSE, MSB, and MSA when either $s_a > 0$ and $s_b > 0$ or $s_a > 0$ and $s_b = 0$.

Proc IML;

use Y; read all into Y;

use X; read all into X;

use A; read all into A;

use B; read all into B;

zero = 0.0000001;

n = nrow(X);

 $Nx = I(n) - X^*ginv(t(X)^*X)^*t(X);$

call eigen(e, Q, Nx);

rankQ = sum(e > zero);

Q = Q[1:n,1:rankQ];

 $Z = t(Q)^*Y;$

* Note E(Z) = 0 and Cov(Z) = v1*Q'*A*A'*Q + v2*Q'*B*B'*Q + v3*I;

* Next compute matrices G and H with full column rank such that ;

*
$$G^*G' = Q'^*A^*A'^*Q$$
 and $H^*H' = Q'^*B^*B'^*Q$;

```
call eigen(e, V, t(Q)^*A^*t(A)^*Q);
```

rankG = sum(e > zero);

V = V[1:n,1:rankG];

D = sqrt(diag(e[1:rankG,1]));

$$G = V^*D;$$

call eigen(e,V, t(Q)*B*t(B)*Q); rankH = sum(e > zero); V = V[1:n,1:rankH]; D = sqrt(diag(e[1:rankH,1])); H = V*D;

* Now calculate the mean squares as described in Section 2.4;

$$L = H^*inv(t(H)^*H);$$

$$N = I(nrow(H)) - L^*t(H);$$

$$U = t(L)^*Z;$$

Atilda = t(L)*G;

$$K = Atilda^*inv(t(Atilda)^*Atilda);$$

$$Nb = I(nrow(Atilda)) - K^*t(Atilda);$$

$$T = t(K)^*U;$$

$$r = rankQ - rankH;$$

$$sb = rankH - rankG;$$

$$ta = rankG;$$

$$MSE = t(Z)^*N^*Z/r;$$

$$MSB = t(U)^*Nb^*U/sb;$$

$$MSA = t(T)^*T/ta;$$

create MSE from MSE; append from MSE;
create MSB from MSB; append from MSB;

create MSA from MSA; append from MSA;

create r from r; append from r;

create sb from sb; append from sb;

create ta from ta; append from ta;

quit;

2.8 Extensions

In this section we consider models with four or more variance components and describe how to calculate the generalized unweighted mean squares for these models.

Suppose $Y \sim MVN_n$ with mean vector and covariance matrix

(8.1) $E(Y) = X\beta$ and $Cov(Y) = \sigma_a^2 V_A + \sigma_b^2 V_B + \sigma_c^2 V_C + \sigma^2 I$ where β , $\sigma^2 > 0$, and σ_a^2 , σ_b^2 , $\sigma_c^2 \ge 0$ are unknown parameters and X, V_A, V_B, and V_C are known matrices such that V_A, V_B, and V_C are n.n.d. Assume $r = n - rank(X, V_A, V_B, V_C)$ is positive, in which case $MSE = Y'(I - P_{(X, V_A, V_B, V_C)})Y/r$ can be defined and has the property $MSE/\sigma^2 \sim \chi^2(r)/r$. Our objective is to define mean squares MSA, MSB, and MSC for model (8.1).

We begin by describing cases where mean squares MSA, MSB, and MSC can be obtained using two variance component methods. For example, if $s_c = rank(X, V_A, V_B, V_C) - rank(X, V_A, V_B)$ is positive then MSC can be defined via two variance component methods. That is, we can transform the data vector to Z = Q'Ywhere Q is any matrix such that $C(Q) = C(X, V_A, V_B)^{\perp}$ and Q'Q = I. Then the resulting model has zero mean and covariance matrix

(8.2)
$$\operatorname{Cov}(Z) = \sigma_{c}^{2} W_{C} + \sigma^{2} I$$

where $W_C = Q'V_CQ$. We can then apply the procedure described in Eubank et al. (1998) to obtain MSC. Similarly, if either $s_b = \operatorname{rank}(X, V_A, V_B, V_C) - \operatorname{rank}(X, V_A, V_C)$ or $s_a = \operatorname{rank}(X, V_A, V_B, V_C) - \operatorname{rank}(X, V_B, V_C)$ is positive then MSB or MSA, respectively, can be obtained using two variance component methods described in Eubank et al. A model where all three mean squares MSC, MSB, and MSA can be defined via two variance component methods is the completely random additive four variance component model:

$$\mathbf{y}_{ijkd} = \boldsymbol{\mu} + \mathbf{a}_i + \mathbf{b}_j + \mathbf{c}_k + \mathbf{e}_{ijkd}.$$

Now if, say, s_a is zero then we cannot convert Y to a two variance component model which depends on σ_a^2 . Instead one would try to convert to a three variance component model and use the procedure described in Section 2.4 to define MSA. Instead of describing this generally, we illustrate this case with the following example.

Example 2.8.3 Öfversten (1993) presented a data set consisting of the yield of two varieties of winter wheat from three locations and two years. He suggested the following model

$$\mathbf{y}_{ijkd} = \boldsymbol{\mu} + \boldsymbol{\tau}_i + \mathbf{a}_j + \mathbf{b}_k + \mathbf{c}_{jk} + \mathbf{e}_{ijkd}$$

 $(i = 1, 2, j = 1, 2, 3, k = 1, 2, and d = 1, ..., n_{ijk})$ where τ_i is the (fixed) effect of variety, and a_j , the random effect of location, b_k , the random effect of year, c_{jk} , the interaction of location and year, and e_{ijkd} , the random error, are mutually independent normal random variables with zero means and variances σ_a^2 , σ_b^2 , σ_c^2 , and σ^2 , respectively. This model can be expressed in matrix form as

$$Y = X\beta + Aa + Bb + Cc + e$$

where X includes both fixed effects.

The mean square MSC can be obtained via two variance component methods. That is, we can convert to $Z_c = Q'_c Y$ where Q_c is any matrix such that $C(Q_c) = C(X, A, B)^{\perp}$ and $Q'_c Q_c = I$. The resulting model is similar to model (8.2) above, and hence, we can define MSC using the procedure described in Eubank et al.

The mean square MSB is obtained using three variance component methods. In particular, one would first calculate $Z_b = Q'_b Y$ where Q_b is any matrix such that $C(Q_b) = C(X, A)^{\perp}$ and $Q'_b Q_b = I$. The resulting model has three components of variance σ_b^2, σ_c^2 , and σ^2 and is completely nested, so we can use the procedure described in 2.4 to obtain MSB. Similarly we can obtain the mean square MSA by transforming the data by Q'_a where Q_a is any matrix such that $C(Q_a) = C(X, B)^{\perp}$ and $Q'_a Q_a = I$. Note that MSC can be alternatively be defined from either Z_b or Z_a using the procedure described in Section 2.4.

The resulting mean squares are MSE = 0.266, MSC = 0.461, MSB = 0.093, and MSA = 1.40 with degrees of freedom r = 8, $s_c = 2$, $t_b = 1$, and $t_a = 2$, respectively. An approximate two-sided confidence interval on $\gamma = k_a \sigma_a^2 + k_b \sigma_b^2 + k_c \sigma_c^2 + k \sigma^2$ for any constants k_a , k_b , k_c , and k can be constructed by replacing the usual ANOVA mean squares in the procedure described in Ting et al. (1990) with mean squares MSA, MSB, MSC and MSE. For example, an interval on $\gamma = \sigma_a^2$ can be obtained by replacing S₁, S₂, S₃, q₁, q₂, and q₃ with MSA, MSC, MSE, t_a , s_c , and r, respectively, in the Ting et al. interval (3.5). The resulting 95% interval on γ is [0, 54.99]. \Box

Next suppose model (8.1) is such that

$$(8.4) C(V_A) \subset C(V_B) \subset C(V_C)$$

and assume s_c , t_b , and $p_a = rank(X, V_A) - rank(X)$ are all positive. For this model, the mean square MSC can be obtained using either two or three variance component methods, similarly to the mean square MSC in the above example. The mean square MSB, however, must be defined via three variance component methods, similarly to MSB in the above example. The resulting mean squares have the properties $MSC/\sigma_c^2 \sim \chi^2(s_c)/s_c$ when $\sigma^2 = 0$ and $MSB/\sigma_b^2 \sim \chi^2(t_b)/t_b$ when $\sigma^2 = \sigma_c^2 = 0$.

Next consider the mean square MSA. To define this mean square we follow the procedure outlined in Section 2.4. That is, first we compute the least squares residuals giving us a completely nested model. Then we mimic the method used to define the unweighted mean squares in the completely random nested classification model with four variance components as described in Section 5.5 of Burdick and Graybill (1992). To illustrate, let Z = Q'Y where Q is any matrix such that $C(Q) = C(X)^{\perp}$ and Q'Q = I and let $q = n - \operatorname{rank}(X)$. Note that $Z \sim MVN_q$ with mean zero and covariance matrix (8.5) $\operatorname{Cov}(Z) = \sigma_a^2 W_A + \sigma_b^2 W_B + \sigma_c^2 W_C + \sigma^2 I$

where $W_A = Q'V_AQ$, $W_B = Q'V_BQ$ and $W_C = Q'V_CQ$ and that $C(W_A) \subset C(W_B) \subset C(W_C)$. Hence, model (8.5) is completely nested. Let A, B, and C be any full rank matrices such that $AA' = W_A$, $BB' = W_B$, and $CC' = W_C$. The unweighted mean square corresponding to MSA in the completely random nested

classification model with four variance components of Burdick and Graybill is based on the means of the means of the cell means and has the property $MSA/\sigma_a^2 \sim \chi^2(p_a)/p_a$ when $\sigma^2 = \sigma_c^2 = \sigma_b^2 = 0$. Imitating this procedure we base MSA on G'Z where $G = KLM, K = C(C'C)^{-1}, \tilde{B} = K'B, L = \tilde{B} (\tilde{B}'\tilde{B})^{-1}, \tilde{A} = L'K'A, and$ $M = \tilde{A} (\tilde{A}'\tilde{A})^{-1}$. Then G'Z ~ MVN_{p_a} with mean zero and $Cov(G'Z) = \sigma_a^2 I + \sigma_b^2 M'M + \sigma_c^2 M'L'LM + \sigma^2 G'G$. Hence, if $\sigma^2 = \sigma_c^2 = \sigma_b^2 = 0$ then there exists a unique quadratic form in G'Z such that $MSA/\sigma_a^2 \sim \chi^2(p_a)/p_a$. For model (8.4), this quadratic from may be expressed as

$$MSA = Z'GG'Z/p_a.$$

It can be shown that MSA satisfies the following properties and that, in fact, these properties uniquely characterize MSA.

- (a) MSA/ $\sigma_a^2 \sim \chi^2(p_a)/p_a$ for all β , $\sigma_a^2 > 0$, and $\sigma_b^2 = \sigma_c^2 = \sigma^2 = 0$;
- (b) MSA and MSE are independent for all β , σ_a^2 , σ_b^2 , σ_c^2 , σ^2 ;
- (c) MSA and MSC are independent for all β , σ_a^2 , σ_b^2 , σ_c^2 , and $\sigma^2 = 0$;
- (d) MSA and MSB are independent for all β , σ_a^2 , σ_b^2 , and $\sigma_c^2 = \sigma^2 = 0$.

It is easy to see how one could further extend the definition of the generalized unweighted mean squares to any P-variance component mixed linear model with a nested covariance structure where $P \ge 5$.

2.9 Concluding Remarks

The unweighted means ANOVA as defined, for example, in Burdick and Graybill (1992) has been extended to the mixed linear model with three variance components, as

well as some models with more than three variance components. The definition of the mean squares from this ANOVA do not require that all cell sample sizes are positive and may be used with covariate or continuous type designs. In fact, the models need not even be classification type models. Additionally they are easy to compute using standard software and can be used with procedures developed by Graybill and Wang (1980) and Ting et al. (1990) to construct confidence intervals on linear combinations of variance components. Simulation studies indicate that the proposed intervals are generally consistent with the stated confidence level. However, for some extremely unbalanced designs the proposed method can produce liberal confidence intervals for some parameter values.

2.10 Proofs

In this section we give the proofs for Propositions 2.5.2 and 2.5.3 from Section 2.5. **Proof of Proposition 2.5.2.** (b) $\Rightarrow C(M) \subset C(X, V_A, V_B)$.

Thus, by (a), (b), and Lemma 2.4 in Seely and Eubank (1998), we have

(i) $\operatorname{rank}(M) = t$

(ii)
$$\mathcal{C}(M) \subset \mathcal{C}(X, V_A, V_B) \cap \mathcal{C}(X)^{\perp}$$

(iii) $M/\sigma_a^2(\sigma_a^2 V_A + \sigma_b^2 V_B)M/\sigma_a^2 = M/\sigma_a^2$ for all $\sigma_a^2 > 0$ and $\sigma_b^2 \ge 0$

(iii)
$$\Rightarrow MV_AM + \sigma_b^2 / \sigma_a^2 V_BM = M \Rightarrow MV_AM = M (by letting \sigma_b^2 = 0)$$

 \Rightarrow M is n.n.d since MV_AM is n.n.d.

Since $MV_AM = M$ then by (iii) we also get, $MV_BM = 0 \Rightarrow V_BM = 0$ (since V_B and M are n.n.d.) $\Rightarrow C(M) \subset C(V_B)^{\perp}$.

Hence,
$$\mathcal{C}(M) \subset \mathcal{C}(X, V_A, V_B) \cap \mathcal{C}(X)^{\perp} \cap \mathcal{C}(V_B)^{\perp} = \mathcal{C}(X, V_A, V_B) \cap \mathcal{C}(X, V_B)^{\perp}$$
 and
rank $(M) = t = \dim \{\mathcal{C}(X, V_A, V_B) \cap \mathcal{C}(X, V_B)^{\perp}\}$

$$\Rightarrow \mathcal{C}(\mathbf{M}) = \mathcal{C}(\mathbf{X}, \mathbf{V}_{\mathbf{A}}, \mathbf{V}_{\mathbf{B}}) \cap \mathcal{C}(\mathbf{X}, \mathbf{V}_{\mathbf{B}})^{\perp}.$$

Similarly if H = H' and R = Y'HY satisfies (a) and (b), then

 $C(H) = C(X, V_A, V_B) \cap C(X, V_B)^{\perp}$. Thus, by Lemma 2.4a and Lemma 2.5 in Seely and Eubank, M = H.

Therefore, M is unique and MSA = Y'MY/t.

We prove the following lemma before establishing Proposition 2.5.3.

Lemma 2.10.1. Suppose M is n.n.d. and satisfies (b) above and let Q be any matrix such that $C(Q) = C(X)^{\perp}$ and Q'Q = I. Then $C(Q'MQ) \subset C(Q'V_BQ)$. Pf. M is n.n.d. $\Rightarrow M = DD'$ for some matrix D and C(M) = C(D). Thus, C(Q'MQ) = C(Q'DD'Q) = C(Q'D). Let $x \in C(Q'D)$. Then x = Q'Dy for some y Now, by (b), $C(D) = C(M) \subset C(X, V_B) = C(V_B) \oplus C(XX'N_B)$ where $N_B = I - P_{V_B}$. So, $D = V_BK + XX'N_BL$ for some matrices K and L. $\therefore x = Q'Ly = Q'(V_BK + XX'N_BL)y = Q'V_BKy \subset C(Q'V_B)$ $\Rightarrow C(Q'MQ) \subset C(Q'V_BQ)$. \Box

Proof of Proposition 2.5.3. By the Lemma 2.3b in Seely and Eubank (1998),

$$\mathcal{C}(MX) \subset \mathcal{C}(X)^{\perp} \Rightarrow X'MX = 0 \Rightarrow X'M = 0 \text{ since } M \text{ is n.n.d.} \Rightarrow \mathcal{C}(M) \subset \mathcal{C}(X)^{\perp}.$$

(b) $\Rightarrow \mathcal{C}(M) \subset \mathcal{C}(X, V_B) \text{ and } (c) \Rightarrow \mathcal{C}(M) \subset \mathcal{C}(V_B(P_{(X,V_B)} - P_{(X,V_A)}))^{\perp}.$
So, $\mathcal{C}(M) \subset \mathcal{C}(X)^{\perp} \cap \mathcal{C}(X, V_B) \cap \mathcal{C}(V_B(P_{(X,V_B)} - P_{(X,V_A)}))^{\perp}.$
Let Q be any matrix such that $\mathcal{C}(Q) = \mathcal{C}(X)^{\perp}$ and $Q'Q = I$, and let A and B be full

column rank matrices such as $AA' = Q'V_AQ$ and $BB' = Q'V_BQ$.

$$\begin{array}{ll} Y'MY &=& Y'QQ'MQQ'Y & \text{since } \mathcal{C}(M) \subset \mathcal{C}(X)^{\perp} \text{ and } QQ' = I - P_X \\ &=& Z'Q'MQZ & \text{where } Z = Q'Y \\ &=& Z'P_BQ'MQP_BZ & \text{since } \mathcal{C}(Q'MQ) \subset \mathcal{C}(Q'V_BQ) = \mathcal{C}(B) \text{ by Lemma 2.9.1} \\ &=& U'KU & \text{where } U = L'Z \text{, } L = B(B'B)^{-1} \text{, and } K = B'Q'MQB \end{array}$$

Now, E(U) = 0 and $Cov(U) = \sigma_a^2 L' A A' L + \sigma_b^2 I + \sigma^2 L' L$

Hence, if $\sigma^2 = 0$ then by Proposition 3.3 in Seely and El-Bassiouni (1983) there exists a

unique quadratic form MSB = U'(I - P_{L'A})U = Y'QL(I - P_{L'A})L'Q'Y such that MSB/ $\sigma_b^2 \sim \chi^2(s)/s$ for some s > 0.

Now
$$C(QL(I - P_{L'A})L'Q') \subset C(QL) = C(QB) = C(QQ'V_BQ) = C((I - P_X)V_B) =$$

 $C(X, V_B) \cap C(X)^{\perp}$ and $QL(I - P_{L'A})L'Q'V_A = 0$ since $C(L'Q'V_A) = C(L'A) \Rightarrow$
 $C(QL(I - P_{L'A})L'Q') \subset C(V_A)^{\perp}.$

Therefore, $\mathcal{C}(QL(I - P_{L'A})L'Q') \subset \mathcal{C}(X, V_B) \cap \mathcal{C}(X, V_A)^{\perp}$. So, by (c), MSB and

Y'MY = U'KU are independent when $\sigma^2 = 0 \implies C(K) \subset C(L'A)$.

Also, (a) $\Rightarrow U'KU/\sigma_a^2 \sim \chi_t^2$ when $Cov(U) = \sigma_a^2 L'AA'L$ and, by Lemma 2.4c in Seely and Eubank, rank(K) = t.

Therefore, by Theorem 2.2 in Seely and Eubank, K = B'Q'MQB is unique.

Hence, if M_1 and M_2 satisfy all of the conditions in the statement of the proposition, then

 $B^\prime Q^\prime M_1 Q B = B^\prime Q^\prime M_2 Q B$

$$\Rightarrow B(B'B)^{-1}B'Q'M_1QB(B'B)^{-1}B' = B(B'B)^{-1}B'Q'M_2QB(B'B)^{-1}B'$$

$$\Rightarrow Q'M_1Q = Q'M_2Q$$
 since $\mathcal{C}(Q'M_iQ) \subset \mathcal{C}(B)$ and $M_i = M'_i$, for $i = 1,2$

$$\Rightarrow QQ'M_1QQ' = QQ'M_2QQ'$$

$$\Rightarrow$$
 M₁ = M₂ since $C(M_i) \subset C(Q)$ and M_i = M', for i = 1,2, and QQ' = P_Q

 \Rightarrow M is unique, and hence, MSA = Y'MY/t. \Box

Confidence Intervals on Variance Components in Mixed Linear Models

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3.1 Abstract

New statistics are developed that can be used for constructing a variance component confidence interval in a three variance component mixed linear model. These statistics are an alternative to the generalized unweighted mean squares in the interval procedure proposed by Ting, Burdick, Graybill, Jeyaratnam, and Lu (1990). This paper presents Monte Carlo simulations that compare the new interval to intervals based on the generalized unweighted and the Type III mean squares. The interval constructed with the new statistics has better coverage probability and is often narrower than the interval constructed with the generalized unweighted mean squares.

3.2 Introduction

Consider the productivity score data presented in Table 23.1 of Milliken and Johnson (1984 p. 285). The experiment was designed to evaluate the productivity of three different brands of machines when operated by the company's own personnel. Six employees from the company were randomly selected to participate in the study and each employee was to operate each machine a given number of times. The response variable is the overall score which is based on the number and quality of components produced. Milliken and Johnson suggested the following two-factor crossed classification model to analyze these data.

(2.1) $y_{ijk} = \mu + \tau_i + \mathbf{a}_j + \mathbf{b}_{ij} + \mathbf{e}_{ijk},$

 $(i = 1, 2, 3, j = 1, ..., 6, \text{ and } k = 1, ..., n_{ij} \ge 0)$ where μ is an unknown constant, τ_i is the (fixed) effect of machine *i*, a_j is the random effect of operator *j*, b_{ij} is the random effect for the machine by operator interaction, and e_{ijk} is the random error. Further, a_j , b_{ij} , and e_{ijk} are mutually independent normal random variables with zero means and

variances σ_a^2 , σ_b^2 , and σ^2 , respectively. Suppose the company is interested in obtaining a confidence interval on the operator to operator variance component σ_a^2 .

Three methods that have been proposed for constructing a confidence interval on σ_a^2 when model (2.1) is balanced are the Satterthwaite method (1946), the Welch method (1956), and the Modified Large Sample (MLS) method of Ting et al. (1990). Each of these methods depends upon the ANOVA mean squares which are independent chi-squared random variables and whose sum is a partition of the error space sum of squares, i.e., the sum of squares of the least squares residuals. However, if model (2.1) is unbalanced, then in most cases there does not exist a set of independent chi-squared random variables whose sum is a partition of the error space.

A technique for constructing confidence intervals in the unbalanced random one-way model was proposed by Thomas and Hultquist (1978). They suggested replacing the usual ANOVA mean squares in the balanced model procedures with mean squares from an unweighted means ANOVA. This idea was extended to other mixed models using unweighted mean squares in the MLS method as though they were mean squares from a balanced ANOVA. This work is summarized in Burdick and Gravbill (1992). A limitation of these procedures is that an unweighted means ANOVA must be available which restricts the class of models that can be accommodated. Eubank, Seely and Lee (1998) showed how to overcome this limitation in two variance component models and in Chapter 2 we extended the Eubank et al. results to more general variance component models. Unfortunately, simulations indicate that for some unbalanced designs the procedures based on the unweighted mean squares or their generalization by Eubank et al. and from Chapter 2, do not maintain the stated confidence level when the intraclass correlation is small. In this paper we develop an alternative set of mean squares that can be used in the MLS method for constructing confidence intervals for variance components. These mean squares are defined for all the models that were

considered in Chapter 2, that is, models where the generalized unweighted mean squares are defined. Our simulation results indicate that the intervals constructed with these new mean squares have better coverage, except possibly for some unusual cases, and are often narrower than other proposed intervals. Additionally these intervals maintain the stated level for small values of the intraclass correlation unlike intervals based on the generalized unweighted mean squares.

We will use the notation C(A) and $C(A)^{\perp}$ to denote the column space of a matrix A and its orthogonal complement, respectively. We will also use the notation A^+ to denote the Moore-Penrose inverse of A and P_A to denote the orthogonal projection operator on the column space of A, i.e., $P_A = A(A'A)^+A'$.

3.3 Existing Methods

Let Y be an n-dimensional multivariate normal (MVN_n) random vector with mean and covariance matrix

(3.1)
$$E(Y) = X\beta \text{ and } Cov(Y) = \sigma_a^2 V_A + \sigma_b^2 V_B + \sigma^2 I_A$$

where β , $\sigma^2 > 0$, σ_a^2 , $\sigma_b^2 \ge 0$ are unknown parameters, X, V_A, V_B are known matrices such that V_A and V_B are nonnegative definite (n.n.d.). Assume that $r = n - rank(X, V_A, V_B)$ is positive. Let $s_a = rank(X, V_A, V_B) - rank(X, V_B)$, $s_b = rank(X, V_A, V_B) - rank(X, V_A)$, and $t_a = rank(X, V_A) - rank(X)$. Consider the problem of constructing a confidence interval on the parameter

(3.2)
$$\gamma = k_a \sigma_a^2 + k_b \sigma_b^2 + k \sigma^2$$

where k_a , k_b , and k are known constants and suppose there exists statistics S_1 , S_2 , and S_3 such that

(3.3) (a)
$$\gamma = E(c_1S_1 + c_2S_2 + c_3S_3)$$
 where c_1, c_2, c_3 are known constants;

(b) $q_i S_i / E(S_i) \sim \chi^2(q_i)$ for i = 1,2,3, where q_1, q_2, q_3 are known integers;

(c) S_1 , S_2 , and S_3 are mutually independent.

Under these assumptions, three methods that have been developed for constructing a confidence interval on γ are the Satterthwaite (1946) method, the Welch (1956) method, and the MLS method of Ting et al. (1990). Based on simulation studies by Ting et al., the MLS method can be recommended. The formula for the Ting et al. MLS interval is given in Section 2.3 of Chapter 2.

If model (3.1) is balanced then it is possible to partition the error sums of squares to obtain mean squares that satisfy conditions (3.3). However, if model (3.1) is unbalanced then generally there does not exist a partitioning that leads to independent chi-squared random variables. Several authors (see, for example, Thomas and Hultquist, 1978, Hernandez and Burdick, 1993a and 1993b, and Hernandez, Burdick, and Birch, 1992) have suggested replacing the S_i s in (3.3) with mean squares from an unweighted means ANOVA and proceeding as though the unweighted mean squares satisfy conditions (3.3). It is well known (see Burdick and Graybill, 1992, p.70), however, that intervals based on the unweighted mean squares can be very liberal for some unbalanced designs. An alternative interval was proposed by Lee, Seely and Purdy (1998) for models with two variance components. Their simulation results indicated that the proposed interval generally maintains the stated confidence level and is often narrower than intervals based on the unweighted mean squares or their generalization. In this paper we extend the method proposed by Lee et al. to the three variance component mixed linear model.

3.4 A New Class of Statistics for Constructing Intervals

Consider model (3.1) and suppose one is interested in constructing a confidence interval on γ in (3.2). Set

(4.1)
$$MSE = Y'(I - P_{(X,V_A,V_B)})Y/r.$$

It is well known that $MSE/\sigma^2 \sim \chi^2(\mathbf{r})/\mathbf{r}$. Note that if $k_a = k_b = 0$, then by standard procedures we can place a confidence interval on γ .

In the next section we develop a class of statistics defined when $s_b > 0$ and demonstrate how one can use a statistic from this class along with MSE to construct confidence intervals on γ when $k_a = 0$. A similar class of statistics was defined by Lee et al. for the two variance component model. Here we show how to extend their definition to model (3.1). The results of Section 3.4.1 can also be used for constructing confidence intervals on γ when $k_b = 0$ and $s_a > 0$ and on γ when both s_a and s_b are positive. Then in Section 3.4.2 we consider the case when either s_a or s_b is equal to zero. Finally in Section 3.4.3, we propose an adaptive interval procedure that utilizes the statistics from the classes defined in the next two sections.

3.4.1 Review of Two-way Methods

Suppose our interest is in determining a confidence interval for γ in (3.2) when $k_a = 0$. That is, on linear combinations of σ_b^2 and σ^2 . Suppose $s_b > 0$ and let $\pi_b = \sigma^2 + \sigma_b^2$ and $\rho_b = \sigma_b^2/\pi_b$. Let Z = C'Y where C is any matrix such that the $C(C) = C(X, V_A)^{\perp}$ and C'C = I. Then $Z \sim MVN$ with zero mean and covariance matrix $Cov(Z) = \sigma_b^2 W_B + \sigma^2 I$ where $W_B = C'V_BC$. Since Z is a two variance component model we can utilize the results of Lee et al. to get a confidence interval for γ when $k_a = 0$. In particular, let G be any full column rank matrix such that $W_B = GG'$, let T = L'Z where $L = G(G'G)^{-1}$ and set

(4.2)
$$MSB(c) = T'\Gamma_c^{-1}T/s_b, \ c \in [0,1],$$

where $\Gamma_c = cI + (1 - c)L'L$. As established in Lee et al., for $c \in [0, 1]$,

(4.3) (a) MSB(c)/ $\pi_b \sim \chi^2(s_b)/s_b$ when $c = \rho_b$;

(b) MSE and MSB(c) are independent.

To verify (a), note that $T \sim MVN(0, \pi_b \Gamma_{\rho_b})$ and that Γ_{ρ_b} is nonsingular of rank s_b . Property (b) follows from the fact that $C(CL) \subset C(X, V_A, V_B)$. Based on properties (4.3) and simulation studies, Eubank, et al. (1998)

recommended using MSB(1) and MSE in the MLS procedure to construct a confidence interval for γ when $k_a = 0$. Other authors, such as Milliken and Johnson (1984), suggest using MSE and the Type III mean square Y'(P_(X,V_A,V_B) - P_(X,V_A))Y/s_b which can be shown to equal MSB(0), and hence, follows a chi-squared distribution when ρ_b is zero. Thus, as one would expect from (4.3a), procedures based on MSB(1) perform well for large values of ρ_b , while procedures based on MSB(0) perform well for small values of ρ_b . As an alternative to using MSB(0) or MSB(1), one might consider using MSB(c) for some value of c in the range (0, 1). For $c \in [0, 1]$, note that

$$E(MSB(c)) = v_c \sigma_b^2 + w_c \sigma^2$$

where

(4.4)
$$\mathbf{v}_{c} = \operatorname{trace}(\Gamma_{c}^{-1})/s_{b}$$
 and $\mathbf{w}_{c} = \operatorname{trace}(\Gamma_{c}^{-1}\Gamma')/s_{b}$.

Then,

(4.5)
$$\hat{\gamma}_{c} = e_{c}MSB(c) + f_{c}MSE$$

where $e_c = k_b/v_c$ and $f_c = k - k_b w_c/v_c$ is unbiased for $\gamma = k_b \sigma_b^2 + k \sigma^2$. Hence, an interval on γ when $k_a = 0$ can then be constructed with MSB(c) and MSE in the MLS interval formula.

Example 3.4.6 Consider the unbalanced case of the productivity score data presented in Table 23.1 of Milliken and Johnson (1984 p. 285) and the suggested model (2.1). We can express model (2.1) in matrix form as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{A}\mathbf{a} + \mathbf{B}\mathbf{b} + \mathbf{e}.$$

where X includes all fixed effects. Then $E(Y) = X\beta$ and $Cov(Y) = \sigma_a^2 V_A + \sigma_b^2 V_B + \sigma^2 I$ where $V_A = AA'$ and $V_B = BB'$. Suppose interest lies in getting a confidence interval on $\gamma = \sigma_b^2$, i.e., $k_a = k = 0$ and $k_b = 1$. There are 44 total observations, three machines, and six operators in the study; hence, $s_b = 10$ and r = 26. Using definitions (4.1) and (4.2), we obtain MSE = 0.87, MSB(0) = 40.43, MSB(0.5) = 21.11, and MSB(1) = 14.50. One approximate confidence interval for γ can be obtained by using MSB(0) and MSE in the MLS method. From (4.4) we get $v_0 = 2.32$ and $w_0 = 1$ for a 95% confidence interval of [8.89; 54.15]. Another approximate interval recommended by Eubank et al. can be obtained using MSB(1), MSE, $v_1 = 1$, and $w_1 = 0.48$. This gives the approximate 95% confidence interval [7.55; 45.15]. An alternative interval could be constructed using MSB(c) for some $c \in (0, 1)$ and MSE. For example, using MSB(0.5) and MSE with $v_{0.5} = 1.37$ and $w_{0.5} = 0.63$ gives the interval [7.12; 47.10]. \Box

If $s_a > 0$, then we can define a class of statistics {MSA(d): $d \in [0, 1]$ } similar to the class {MSB(c): $c \in [0, 1]$ } by simply interchanging the roles of V_A and V_B and following the procedure in (4.2). An approximate interval on γ in (3.2) when $k_b = 0$ can then be constructed with MSE and MSA(d) in the MLS procedure. Additionally, an interval on γ , for any k_a , k_b , and k, can be constructed with MSE, MSB(c) and MSA(d) when both s_a and s_b are positive.

However, if $s_a = 0$ (or $s_b = 0$) then we cannot use the procedure described above to obtain a class of statistics corresponding to $\sigma_a^2 (\sigma_b^2)$ since there does not exist a transformation of the data that gives us a model with only two variance components, one being $\sigma_a^2 (\sigma_b^2)$. Hence, we need to define a new class of estimators. In the next section we consider the case when $s_a = 0$ and define a new class of statistics that can be used with the statistics MSB(c) and MSE to construct intervals for any γ in (3.2).

3.4.2 Three-way Methods

Recall that if both s_a and s_b are positive, then a confidence interval for any γ in (3.2) can be constructed from the two-way methods of the previous section. Thus, let us consider the case when $s_a = 0$ and $s_b > 0$ and suppose interest is in placing a confidence interval on γ . If $k_a = 0$ then an interval can be constructed using MSB(c) and MSE as

described in the previous section. A problem occurs when $k_a \neq 0$. In this section we will develop a new class of statistics that can be used along with MSB(c) and MSE to construct confidence intervals on γ when $k_a \neq 0$.

To proceed we assume that t_a is positive. Let $\pi = \sigma^2 + \sigma_b^2 + \sigma_a^2$ and $\eta_a = \sigma_a^2/\pi$ and recall the definitions of π_b and ρ_b from the previous section. Following the procedure outlined in Section 2.4.2 of Chapter 2, let Z = Q'Y where Q is any matrix such that the columns of Q form an orthonormal basis for C(X). Then $Z \sim MVN$ with zero mean and covariance matrix $Cov(Z) = \sigma_a^2 W_A + \sigma_b^2 W_B + \sigma^2 I$ where $W_A = Q'V_AQ$, $W_B = Q'V_BQ$. Since $s_a = 0$, it follows that $C(V_A) \subset C(X, V_B)$ which implies $C(W_A) \subset C(W_B)$. Let H and G be any full column rank matrices such that $W_A = HH'$ and $W_B = GG'$. Let U = K'L'Z where $L = G(G'G)^{-1}$, $K = \widetilde{H} (\widetilde{H}'\widetilde{H})^{-1}$, and $\widetilde{H} = L'H$. For c, $d \in [0, 1]$, set (4.7) MSA(c, d) = U'\Lambda_c^{-1}U/t_a

where $\Lambda_{c,d} = dI + c(1 - d)K'K + (1 - c)(1 - d)K'L'LK$. MSA(1, 1) is equal to the statistic MSA in (4.12) of Chapter 2, and hence, has the properties given in Proposition 2.5.3 of Section 2.5. It can be shown that for fixed c and d, MSA(c, d) has similar properties. In particular, if c, $d \in [0,1]$, then

(4.8) (a) MSA(c,d)/
$$\pi \sim \chi^2(t_a)/t_a$$
 when $\rho_b = c$ and $\eta_a = d$;

- (b) MSE and MSA(c,d) are independent;
- (c) MSB(c) and MSA(c,d) are independent when $\sigma^2 = 0$.

Part (a) follows from the fact that $U \sim MVN(0, \pi \Lambda_{\rho_b, \eta_a})$ and rank $(\Lambda_{\rho_b, \eta_a}) = rank(\widetilde{H}) = t_a$. Property (b) follows since $C(QLK) \subset C(QL) \subset C(X, V_B)$ and (c) follows since $C(QLK) \subset C(V_B(I - P_{(X,V_A)}))^{\perp}$.

Now suppose one is interested in constructing a confidence interval on γ in (3.2). Observe that

$$E(MSA(c,d)) = g_{c,d}\sigma_a^2 + h_{c,d}\sigma_b^2 + k_{c,d}\sigma^2$$

where

(4.9)
$$g_{c,d} = \operatorname{trace}(\Lambda_{c,d}^{-1})/t_a, \qquad h_{c,d} = \operatorname{trace}(K\Lambda_{c,d}^{-1}K')/t_a,$$

and

$$k_{c,d} = trace(LK\Lambda_{c,d}^{-1}K'L')/t_a$$

An unbiased estimator of γ can be obtained with MSE, MSB(c) and MSA(c,d). In particular, let

(4.10)
$$\widehat{\gamma}_{c,d} = m_{c,d}MSA(c,d) + n_{c,d}MSB(c) + p_{c,d}MSE$$

where

$$\mathbf{m}_{\mathsf{c},\mathsf{d}} = k_{\mathsf{a}}/g_{\mathsf{c},\mathsf{d}}, \quad \mathbf{n}_{\mathsf{c},\mathsf{d}} = (k_b \mathbf{g}_{\mathsf{c},\mathsf{d}} - k_a \mathbf{h}_{\mathsf{c},\mathsf{d}})/(\mathbf{g}_{\mathsf{c},\mathsf{d}} \mathbf{v}_{\mathsf{c}}),$$

and

$$\mathbf{p}_{\mathsf{c},\mathsf{d}} = k + \left[k_a (\mathbf{h}_{\mathsf{c},\mathsf{d}} \mathbf{w}_{\mathsf{c}} - \mathbf{k}_{\mathsf{c},\mathsf{d}} \mathbf{v}_{\mathsf{c}}) - k_b \mathbf{g}_{\mathsf{c},\mathsf{d}} \mathbf{w}_{\mathsf{c}} \right] / (\mathbf{g}_{\mathsf{c},\mathsf{d}} \mathbf{v}_{\mathsf{c}})$$

with v_c and w_c defined in (4.4). Then $\hat{\gamma}_{c,d}$ is unbiased for γ and an interval on γ can then be constructed by using MSA(c,d), MSB(c), and MSE in the MLS procedure.

Example 3.4.6 (Continued): Using definition (4.7), we obtain

MSA(0,0) = 201.75, MSA(0.5, 0.5) = 44.22, and MSA(1,1) = 27.36. For c, d = 0, 0.5, 1, coefficients (4.9) are $g_{0,0} = 7.22$, $h_{0,0} = 2.59$, $k_{0,0} = 1$, $g_{0.5,0.5} = 1.60$, $h_{0.5,0.5} = 0.53$, $k_{0.5,0.5} = 0.26$, $g_{1,1} = 1$, $h_{1,1} = 0.333$, and $k_{1,1} = 0.160$. Based on (4.10), two unbiased estimates of $\gamma = \sigma_a^2$ are $\hat{\gamma}_{0,0} = 21.44$ and $\hat{\gamma}_{1,1} = 22.23$. A 95% confidence interval on γ based on MSA(0,0), MSB(0) and MSE in the MLS methods is [0.77; 161.43]. The MLS interval based on MSA(1,1), MSB(1) and MSE is [3.47; 159.41] and the interval based on MSA(0.5, 0.5), MSB(0.5) and MSE is [2.93; 160.26]. \Box

3.4.3 The Adaptive Interval

As mentioned previously, confidence intervals for γ in (3.2) based on MSA(0,0) and MSB(0) have good coverage probabilities for small values of η_a and ρ_b , but the intervals tend to be liberal for larger values of η_a and ρ_b . Similarly intervals based on MSA(1,1) and MSB(1) perform well for η_a and ρ_b near one, but for some unbalanced designs the intervals are too liberal for small values of η_a and ρ_b . To get better probability coverage for all values of η_a and ρ_b , we follow Lee et al. (1998) and use an adaptive approach that allows the data to select the values of c and d. In particular, we recommend using

 $MSA(\hat{\rho}_b, \hat{\eta}_a)$ and $MSB(\hat{\rho}_b)$ where $\hat{\eta}_a$ and $\hat{\rho}_b$ are estimators for η_a and ρ_b , respectively.

Consider the class of estimators for η_a defined by

$$\widehat{\eta}_{a}(c,d) = \widehat{\gamma}_{c,d}^{+} / \left(\widehat{\gamma}_{c,d}^{+} + \widehat{\gamma}_{c}^{+} + MSE \right)$$

and the class of estimators for $\rho_{\rm b}$ defined by

$$\hat{\rho}_{b}(c) = \hat{\gamma}_{c}^{+} / (\hat{\gamma}_{c}^{+} + MSE),$$

where $\hat{\gamma}_{c,d}^+ = \max\{0, \hat{\gamma}_{c,d}\}, \ \hat{\gamma}_c^+ = \max\{0, \hat{\gamma}_c\}, \ \hat{\gamma}_{c,d}$ is the estimator of σ_a^2 given by (4.9) (i.e., by setting $k_a = 1, k_b = 0$, and k = 0), and $\hat{\gamma}_c$ is the estimator of σ_b^2 given by (4.5) (i.e., by setting $k_b = 1$ and k = 0). We considered different estimators of η_a and ρ_b from these classes and found that intervals based on $\hat{\eta}_a(0,0)$ and $\hat{\rho}_b(0)$ performed the best over the complete range of parameter values. Therefore we propose constructing intervals with MSA($\hat{\rho}_b, \hat{\eta}_a$), MSB($\hat{\rho}_b$), and MSE in the MLS method where $\hat{\eta}_a =$ $\hat{\eta}_a(0,0)$ and $\hat{\rho}_b = \hat{\rho}_b(0)$.

Example 3.4.6 (Continued): An additional confidence interval on $\gamma = \sigma_a^2$ can be obtained using MSA($\hat{\rho}_b$, $\hat{\eta}_a$) and MSB($\hat{\rho}_b$) in the MLS method where $\hat{\eta}_a = \hat{\eta}_a(0,0) = 0.547$ and $\hat{\rho}_b = \hat{\rho}_b(0) = 0.951$. These estimates give MSB($\hat{\rho}_b$) = 14.95 and MSA($\hat{\rho}_b$, $\hat{\eta}_a$) = 39.42. The computed 95% confidence interval on γ is [3.43; 159.47]. \Box

3.5 Simulation Results

In this section we give simulation results for three confidence intervals on σ_a^2 in model (3.1) when $s_a = 0$ and $s_b > 0$. We obtained simulation results for other designs, but the examples below illustrate the general properties of each method. The performance of the confidence interval procedures is measured by coverage probability and average interval length. All of the reported intervals are two-sided 95% confidence intervals with equal tail probability. We also ran simulations for 99% confidence intervals and found that the performance of these intervals was similar to the 95% confidence intervals, and hence, the results are not reported. Similarly, we considered other linear combinations of σ_a^2 , σ_b^2 , and σ^2 , and found the results to be similar to those given here. For each design we considered several values of η_a and ρ_b ; specifically, $\eta_a = 0.01, 0.25, 0.5, 0.75, 0.99$ and $\rho_b = 0.01, 0.5, 0.99$. The simulation results are based on 2000 pseudo-random data sets generated in S-PLUS. This results in a standard error of approximately 0.5% on the coverage probabilities given in the tables below.

The three methods reported are MLS(0,0) which is the MLS method using Type III mean squares, MLS(1,1) which is the MLS method using MSE, MSB(1), and MSA(1, 1), and MLS($\hat{\rho}_b$, $\hat{\eta}_a$) which is the MLS method using the adaptive statistics MSE, MSB($\hat{\rho}_b$), and MSA($\hat{\rho}_b$, $\hat{\eta}_a$) defined in the previous section. Note that for the models and designs where an unweighted means ANOVA can be constructed, MSB(1) and MSA(1, 1) are the unweighted mean squares defined in Burdick and Graybill (1992). For models or designs where the unweighted means ANOVA is not defined, MSB(1) and MSA(1, 1) are the generalized unweighted mean squares from Chapter 2.

Example 3.5.1 Consider the unbalanced case of the productivity score data presented in Table 23.1 of Milliken and Johnson (1984 p. 285) and the recommended model

(5.2)
$$y_{ijk} = \mu + \tau_i + a_j + b_{ij} + e_{ijk},$$

 $(i = 1, 2, 3, j = 1, ..., 6, k = 1, ..., n_{ij})$ where μ and τ_i are fixed effects and a_j , b_{ij} , and e_{ijk} are mutually independent normal random variables with zero means and variances σ_a^2 , σ_b^2 , and σ^2 , respectively. For this data set $n_{11} = n_{13} = n_{21} = 1$, $n_{12} =$ $n_{14} = n_{23} = n_{25} = 2$, and the remaining n_{ij} are equal to 3. The degrees of freedom are $t_a = 5$, $s_b = 10$, and r = 26. The confidence coefficients for intervals on σ_a^2 are given in Table 3.1. The coefficients for other intermediate values of η_a and ρ_b were similar to those given in the table, and hence, were omitted. Clearly, this design is not very unbalanced. Thus, it is not surprising that all three methods maintain the stated level. Additionally, the average interval widths are very similar for each of the methods. \Box

Table 3.1 Confidence coefficients for intervals on σ_a^2 in Example 3.5.1 with stated level of 95%

η_{a}	$ ho_{ m b}$	MLS(0,0)	MLS(1,1)	$\mathrm{MLS}(\widehat{\rho}_{\mathrm{b}},\widehat{\eta}_{\mathrm{a}})$
0.01	0.01	94.65	94.70	95.05
	0.50	95.25	94.60	94.80
	0.99	94.70	94.55	94.55
0.50	0.01	95.50	95.85	95.70
	0.50	95.25	95.60	95.65
	0.99	93.95	95.10	95.10
0.99	0.01	94.40	94.95	94.95
	0.25	94.80	95.05	95.05
	0.99	95.00	95.65	95.65

Example 3.5.3 Consider model (5.2) from Example 3.5.1 and let

 $n_{11} = n_{12} = n_{21} = n_{23} = n_{25} = n_{35} = 0$, $n_{16} = n_{26} = n_{36} = 10$, and all the remaining n_{ij} equal to 2. The degrees of freedom for this design are $t_a = 5$, $s_b = 4$, and r = 36. The simulation results are summarized in Table 3.2. For this design we find that the MLS interval with the generalized unweighted mean squares are slightly liberal when η_a is small but for the other parameter values it maintains the stated level. The MLS method based on the Type III mean squares gave very liberal intervals for large values of η_a , whereas the adaptive interval maintained the stated level for all parameter values. Also we found that for small values of η_a , particularly $\eta_a = 0.01$ and 0.25, the proposed

Table 3.2 Confidence coefficients for intervals on σ_a^2 in Example 3.5.3 with stated level of 95%

η_{a}	$ ho_{ m b}$	MLS(0,0)	MLS(1,1)	MLS($\hat{\rho}_{b}, \hat{\eta}_{a}$)
0.01	0.01	94.95	93.15	95.20
	0.50	94.50	93.05	94.85
	0.99	94.75	93.70	94.85
0.50	0.01	91.60	95.50	94.75
	0.50	93.85	96.05	95.70
	0.99	93.60	95.20	95.30
0.99	0.01	91.15	94.55	94.55
	0.25	89.45	94.30	94.35
	0.99	89.95	95.05	95.05

intervals MLS($\hat{\rho}_b, \hat{\eta}_a$) were 20% to 30% narrower than the intervals based on the generalized unweighted mean squares. \Box

Example 3.5.4 Consider the following completely random nested model (5.5) $y_{ijk} = \mu + a_i + b_{ij} + e_{ijk}$ $(i = 1, ..., I, j = 1, ..., m_i, k = 1, ..., n_{ij})$ where a_i, b_{ij} , and e_{ijk} are mutually

independent normal random variables with zero means and variances σ_a^2 , σ_b^2 , and σ^2 , respectively. Consider a design with I = 5, $m_i = 20$ for i = 1, ..., 4, $m_5 = 1$, and $n_{ij} = 2$ for all *i*, *j*. Then the degrees of freedom are $t_a = 4$, $s_b = 76$, and r = 81. The simulation results, presented in Table 3.3, indicate that for this design the proposed method MLS($\hat{\rho}_b$, $\hat{\eta}_a$) maintains the stated level for the complete range of the parameter

η_{a}	$ ho_{ m b}$	MLS(0,0)	MLS(1,1)	$\mathrm{MLS}(\widehat{\rho}_{\mathrm{b}},\widehat{\eta}_{\mathrm{a}})$
0.01	0.01	94.50	86.80	94.05
	0.50	94.75	84.05	94.40
	0.99	95.10	83.75	94.85
0.50	0.01	91.65	93.35	93.80
	0.50	91.80	93.95	93.90
	0.99	92.85	94.60	94.60
0.99	0.01	92.10	94.85	94.70
	0.25	92.65	95.50	94.80
	0.99	91.50	95.45	94.45

Table 3.3 Confidence coefficients for intervals on σ_a^2 in Example 3.5.4 with stated level of 95%

values. However, the intervals based on the generalized unweighted mean squares MLS(1,1) are very liberal for small values of η_a and the intervals based on the Type III mean squares MLS(0,0) are quite liberal for large values of η_a . Additionally, for small values of η_a , the intervals based on the adaptive statistics are significantly narrower than intervals based on the generalized unweighted mean squares. In particular, when $\eta_a = 0.01$ and $\rho_b = 0.01$, 0.25, and 0.99, the ratios of the average lengths of the MLS($\hat{\rho}_b, \hat{\eta}_a$) interval to the MLS(1,1) interval are 0.389, 0.383, 0.356, indicating that the proposed interval is approximately one-third the width of the MLS interval with the generalized unweighted mean squares. As η_a approaches one the two intervals have similar probability coverage and width. \Box

Example 3.5.6 Consider model (5.5) from Example 3.5.3 and let I = 7, $m_i = 2$ for i = 1, ..., 5, $m_6 = 100$, and $n_{ij} = 2$ for all i, j. The degrees of freedom for this design are $t_a = 6$, $s_b = 49$, and r = 56. The simulation results are given in Table 3.4. Once again the adaptive interval generally maintains the stated level and has better coverage than either of the other two methods. For this design we find the intervals based on the Type III mean squares to be very liberal for large values of ρ_b and the intervals based on the generalized unweighted mean squares to be slightly liberal for small values of η_a . Additionally, the adaptive interval is approximately 25% narrower than the interval based on the generalized unweighted mean squares for small values of η_a and it has approximately the same width as the interval based on the Type III mean squares. \Box

We considered other designs similar to those in Examples 3.5.4 and 3.5.6 and obtained comparable results. In particular, we found that for designs where there are several large groups and only a few small groups, as in Example 3.5.4, the MLS interval with the Type III mean squares can be moderately liberal for large values of η_a while the

η_{a}	$ ho_{ m b}$	MLS(0,0)	MLS(1,1)	$\mathrm{MLS}(\widehat{\rho}_{\mathfrak{b}},\widehat{\eta}_{\mathfrak{a}})$
0.01	0.01	94.15	92.85	93.90
	0.50	94.95	93.25	94.05
	0.99	95.45	94.15	94.80
0.50	0.01	90.75	94.15	93.20
	0.50	91.25	95.30	94.75
	0.99	91.55	94.40	93.15
0.99	0.01	88.80	94.70	94.55
	0.25	88.90	95.50	94.50
	0.99	88.60	95.00	94.70

Table 3.4 Confidence coefficients for intervals on σ_a^2 in Example 3.5.6 with stated level of 95%

MLS interval with the generalized unweighted mean squares are very liberal for small values of η_a . For designs with several small groups and a few large groups, as in Example 3.5.6, the MLS interval with the generalized unweighted mean squares can be slightly liberal for small values of η_a and the Type III interval can be very liberal for large values of η_a . However, for all of these designs we found that the interval based on the adaptive statistics is almost always consistent with the stated level and for small values of η_a it is narrower than the MLS interval based on the generalized unweighted mean squares.

3.6 Alternative Expressions

Consider model (3.1). Let A and B be any matrices such that $V_A = AA'$ and $V_B = BB'$. In this section we give alternative expressions for MSB(c) and MSA(c,d) that involve only X, A and B, and hence, are easier to calculate than the expressions given in Section 3.4. To demonstrate that the new expressions are equivalent to the formulas given in Section 3.4 we first state two propositions.

Recall that $\pi = \sigma^2 + \sigma_b^2 + \sigma_a^2$, $\pi_b = \sigma^2 + \sigma_b^2$, $\eta_a = \sigma_a^2/\pi$, and $\rho_b = \sigma_b^2/\pi_b$. Before we state the first proposition, observe that the covariance matrix of Y can be parameterized via π_b and ρ_b . With this parameterization, Cov(Y) may be expressed as $Cov(Y) = \sigma_a^2 V_A + \pi_b (\rho_b V_B + (1 - \rho_b)I)$. We use this parameterization when proving the following proposition.

Proposition 3.6.1 Let $c \in [0, 1]$ and suppose M is a symmetric matrix such that (a) $Y'MY/\pi_b \sim \chi^2(s_b)$ when $\rho_b = c$ for all β and $\pi_b > 0$; (b) $C(M) \subset C(X,B)$.

Then M is unique, and hence, $MSB(c) = Y'MY/s_b$ by (4.3).

Now observe that the covariance matrix of Y can be parameterized via π , η_a and ρ_b . With this parameterization, Cov(Y) may be expressed as Cov(Y) = $\pi (\eta_a V_A + \rho_b (1 - \eta_a) V_B + (1 - \rho_b) (1 - \eta_a) I)$. Again, this parameterization

is used to prove the following proposition.

Proposition 3.6.2 Let c, $d \in [0, 1]$ and assume N is a nonnegative definite matrix such that

(a)
$$Y'NY/\pi \sim \chi^2(t_a)$$
 when $\rho_b = c$ and $\eta_a = d$ for all β and $\pi > 0$;

(b)
$$\mathcal{C}(N) \subset \mathcal{C}(X,B);$$

(c) $\text{Cov}(NY, (P_{(X,B)} - P_{(X,A)})Y) = 0$ when $\sigma^2 = 0$.

Then N is unique, and hence, $MSA(c,d) = Y'NY/t_a$ by (4.8).

The proofs for Propositions 3.6.1 and 3.6.2 are similar to the proofs for

Propositions 2.5.2 and 2.5.3, respectively, in Chapter 2.

Let
$$Z = L'Y$$
 where $L = (I - P_X)B$. For $c \in [0, 1]$, set

$$M(c) = Z'V_c^{\dagger}Z/s_b$$

where $V_c = c(L'L)^2 + (1 - c)L'L$. It is easy to check that M(c) satisfies (a) and (b) in Proposition 3.6.1. Hence, the proposition implies M(c) = MSB(c) in (4.2).

Let U=K'Y where $K=\big[(I-P_H)X,(I-P_H)B\big]$ and $H=(X,\,BB'(I-P_{(X,A)})).$ For c, $d\in[0,\,1],$ set

$$N(c,d) = U'T_{c,d}^+U/t_a$$

where $T_{c,d} = dK'AA'K + c(1 - d)K'BB'K + (1 - c)(1 - d)K'K$. It can be easily shown that N(c,d) satisfies (a)-(c) in Proposition 3.6.2. Hence, N(c,d) = MSA(c,d) in (4.7).

3.7 Concluding Remarks

A set of statistics has been defined for constructing confidence intervals in three variance component mixed linear models. These statistics can be used as an alternative to the generalized unweighted mean squares in the MLS method and are easy to compute using standard software. Simulation studies indicate that the proposed interval has better coverage than intervals based on either the generalized unweighted or Type III mean squares. Additionally, the proposed interval is often narrower than the interval based on the generalized unweighted mean squares.

Chapter 4

Summary

This thesis considers the problem of constructing confidence intervals on variance components in mixed linear models. In Chapter 2 of this thesis we generalized the unweighted means ANOVA to mixed models with more than two variance components. The mean squares from this ANOVA are defined for three variance component models, as well as, some models with more than three variance components. The definitions do not require that all cells are nonempty and allows for covariates. Under mild rank restrictions, these mean squares can be employed in the Modified Large Sample (MLS) procedure to construct confidence intervals on any linear combinations of variance components and are easy to compute using standard software. Simulation studies indicated that the MLS intervals with the generalized unweighted mean squares are usually consistent with the stated confidence level. However, for some extremely unbalanced designs these intervals may be quite liberal.

In Chapter 3 we defined a set of adaptive statistics for constructing confidence intervals in three variance component mixed linear model. These statistics can be used as an alternative to the unweighted mean squares in the MLS method and are also easy to compute using standard software. Simulation studies indicate that the proposed interval has better coverage than intervals based on either the generalized unweighted or Type III mean squares. Additionally, the proposed interval is often narrower than the interval based on the generalized unweighted mean squares.

The method in Chapter 3 also shows promise for testing variance components. Preliminary findings indicate that this method gives highly accurate results and has better power than some exact tests (e.g., Christensen 1996, Khuri and Littell 1987) that are non-unique.

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