A GENERAL SOLUTION TO MAKING INFERENCES ABOUT THE PARAMETERS OF MIXED LINEAR MODELS

By

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CHAPTER I

INTRODUCTION

One of the most challenging problems in statistics is estimating the variance components of mixed linear models. This study presents a Bayesian estimation procedure for estimating these parameters, as it describes a general solution for balanced and unbalanced designs.

The mixed model considered in this study is

$$y = x\theta + ub + e \quad , \tag{1.1}$$

where:

- y is an $Nx1$ random vector whose observed values comprise the data points,
- x is a Nxp full rank $(N > p)$ known design matrix,
- θ is a $px1$ unknown real parameter vector,
- u is a Nxm known design matrix,
- b is a $mx1$ unknown random vector, and
- e is a $Nx1$ unknown random error vector.

The matrix u is partitioned as

$$(u_1, u_2, \ldots, u_c) \quad ,$$

where u_i is a Nxm_i full rank, and b' is partitioned as

$$(b_1', b_2', \ldots, b_c') \quad ,$$

where b_i is a $m_i \times 1$ normal random vector with mean vector zero and dispersion matrix

$$D(b_i) = \sigma_i^2 I_{m_i} \quad , \quad i = 1, 2, \ldots, c \quad ,$$

and

$$m = \sum_{i=1}^{c} m_i \quad .$$

The error vector e is normal with mean vector zero and dispersion matrix

$$D(e) = \sigma^2 I_N \quad .$$

The random vectors $b_1, b_2, \ldots, b_c$ are assumed to be independent and each to be independent of e.

The components of the parameter vector θ are called the fixed effects, and the components of the random vector b are called the random effects. The error variance is σ^2 and the variances components are $\sigma_1^2, \sigma_2^2, \ldots, \sigma_c^2$.

The objective of this study is to estimate the parameters of the mixed model 1.1, as well as τ and τ_i , where

$$\tau = \sigma^{-2} \quad ,$$

$$\tau_i = \sigma_i^{-2} \quad , \quad i = 1, 2, \ldots, c \quad .$$

The following Bayesian approach will be used.

1. Determine an estimator for the random effects, b. The least square estimator, b^*, will be used as a conditioning value in the following stages.

2. Determine the conditional posterior distribution of the fixed effects θ, given b^*. The conditional posterior mean of θ

given b^* will be denoted by Θ^* .

3. Determine the conditional posterior distribution of the variance components given b^* and Θ^*. The conditional mean of this conditional distribution will be considered as an estimate of the variance components.

The organization of this thesis is as follows: the literature pertaining to classical and Bayesian approaches for estimating variance components is reviewed in Chapter II. In Chapter III, the general derivations concerning the posterior distributions are presented. The thesis is then briefly summarized and recommendations for further research are presented in Chapter IV. A discussion of a simple numerical algorithm using SAS(1) is presented in the appendix.

CHAPTER II

LITERATURE REVIEW

In the non-Bayesian methods for estimating the variance components, one must find the sampling distribution of the estimators, which is not always an easy task. Also, computational difficulties are the disadvantage of some non-Bayesian as well as Bayesian approaches.

Analysis of Variance

The most popular non-Bayesian methods for estimating variance components are methods I, II, and III; by Henderson (8). Searle (14) gives an excellent description of Henderson's methods and indicated various generalizations. In these methods, mean squares associated with various analysis of variance tables are set equal to their expectations and the estimators are obtained by solving the resulting equations. These methods yield translation invariant quadratic unbiased estimators. However, these quadratic forms are functionally independent of the variance components, the expectations are linear, and negative estimators of variance components can be realized.

With Henderson's method I for unbalanced data, expressions for the sum of squares are established by analogy with the analysis of variance of balanced data. Next the expectations of all such analogous expressions are computed and are equated to their expectations and solved for the unknown variances. This method can be used only for random models, because in mixed models the expected values of the sums of squares terms contain functions of the fixed effects. These functions cannot be eliminated by considering linear combinations of the analysis of variance sums of squares.

In Henderson's method II, one first estimates the fixed effects by least squares assuming that the overall mean of the model is zero and that the random effects are fixed. Then, the data is corrected according to the estimates of the fixed effects, and using the corrected data in place of the original data, one proceeds as in method I. This method provides unbiased estimators, but as has been shown by Searle (15), the method is not uniquely defined and it cannot be used whenever the model includes interactions between the fixed and the random effects.

The last of these methods is the method of fitting constants or Henderson's method III. The method uses reductions in the sums of squares to fit the full and reduced models. The reductions are used in the same manner as the sums of squares terms, namely estimating variance components by equating each computed reduction to its expected value under the full model. This method yields unbiased variance component estimators.

Maximum Likelihood

Unlike least squares, maximum likelihood estimation uses some assumptions about the distribution of the random error term in the model. In general, the maximum likelihood estimates are obtained by taking the partial derivatives of the likelihood function or its logarithm with respect to the components of the parameter vector, and by equating them to zero to obtain the likelihood equations. If these equations have a unique solution, it must be the true maximum likelihood estimate. In some complicated estimation problems, the likelihood equations may have multiple roots, and/or the roots may or may not lie in the parameter space. In such cases, it is necessary to obtain solutions along the boundaries of the parameter space and compare their values to obtain the maximum likelihood estimators. This method received little attention until recently because the complexity of the likelihood equations. Numerical techniques for the solution of the likelihood equations have been discussed by Hartly and Rao (5). They proposed a computational algorithm for the solution of the likelihood equation and proved that under certain restrictions the estimates were consistent and asymptotically normal as the size of the experimental design increased.

Restricted Maximum Likelihood

Patterson and Thompson (10), considered the general linear model

$$y = x\theta + e \quad ,$$

in which $e \sim N(o, \sigma^2 H)$. They partitioned the data vector y into two vectors which produces two logarithmic likelihoods, L_1 and L_2. Then, they estimated the variance components by maximizing L_1 and estimated θ by maximizing L_2. The two vectors can be represented by Sy and Qy with the following properties:

1. The matrix S, which may be represented by

$$I - x(x'x)^{-1}x' \quad ,$$

is of rank $N-p$, where x is at full rank p. This implies that

$$Sx = 0$$

and therefore

$$E(Sy) = 0.$$

2. The matrix Q, which may be represented by

$$x'H^{-1} \quad ,$$

as well as the matrix Qx is of full rank p. Every linear function of the elements of Qy estimates a linear function of the elements of θ.

3. The two vectors, Sy and Qy, are statistically independent, because

$$SHQ' = 0 \quad .$$

Corbeil and Searle (3) adapted Patterson and Thompson's procedure and developed another procedure which is applicable to mixed models for any mix of fixed and random effect. They avoid the singularity of SHS by deleting some rows from the matrix S to get another transformation matrix, T. The matrix T has the following properties:

1. $Tx = 0$, and therefore

$$E(Ty) = 0 \quad ,$$

2. $T'(TT')^{-1}T = S$.

Minimum Norm Quadratic Unbiased Estimators - MINQUE

Rao (11) suggested estimating a linear function of the variance components

$$Q = \sum_{i=1}^{c+1} p_i\sigma_i^2$$

by a quadratic function

$$y'Ay$$

of the random variable y. He proposed the estimator

$$y'A^{*}y \quad ,$$

where A^{*} minimizes the norm

$$||\omega'A\omega - \Delta||$$

for A such that $y'A^{*}y$ is a translation-invariant quadratic unbiased estimator of Q. Here

$$\omega' = (b', e') \quad ,$$

$$\frac{p_{c+1}}{N} e'e + \sum_{i=1}^{c} \frac{p_i}{m_i} b_i'b_i = (b', e') \; \Delta \binom{b}{e} \quad , \qquad \text{and}$$

$||\cdot||$ denotes a matrix norm.

Minimum Variance Quadratic Unbiased

Estimator - MIVQUE

Rao (12) developed the MIVQUE theory. He considered the MIVQUE of a linear combination of the variance components as a quadratic form $y'Ay$, which is similar to that in MINQUE, where A is chosen to minimize the variance of $y'Ay$. The MINQUE of Q (based on Euclidean norm) is the same as the MIVQUE (derived on the basis of the normality assumption). Swallow and Searle (16) obtained a MIVQUE of variance components from unbalanced and balanced data obtained for the one-way classification random model under normality. They also made a comparison between the MIVQUE and the analysis of variance estimators.

Bayesian Approach

Lindley and Smith (9) argued, within the Bayesian framework, that prior information is available about the parameters of a model. Their technique amounts to expressing the fixed effects in the original model as a deviation from hyperparameters, expressing the hyperparameters as deviations from hyper-hyperparameters, or second-order hyperparameters; expressing second-order hyperparameters as deviations from third-order hyperparameters, etc. In the redefined model, the highest order hyperparameters comprise the components of the fixed effects and the components of the random effects. They considered the model

$$E(y) = A_1\theta_1 .$$

The likelihood function is

$$y|\theta_1 \sim N(A_1\theta_1, C_1) \quad ;$$

and the marginal distribution of θ_1 is:

$$\theta_1 \sim N(A_2A_3\theta_3, C_3 + A_2C_3A_2') \quad ,$$

where

$$\theta_1|\theta_2 \sim N(A_2\theta_2, C_2) \quad .$$

and

$$\theta_2|\theta_3 \sim N(A_3\theta_3, C_3).$$

This leads to the posterior distribution of θ_1, given $\{A_i\}$, $\{C_i\}$, θ_3 and y, which is $N(Dd, D)$ with

$$D^{-1} = A_1'C_1^{-1}A_1 + \{C_2 + A_2C_3A_2'\}^{-1}$$

and

$$d = A_1'C_1^{-1}y + \{C_2 + A_2C_3A_2\}^{-1}A_2A_3\theta_3 .$$

The mean of this posterior distribution is considered to be a point estimate of θ_1. That estimate is the weighted average of the least squares estimate

$$(A_1'C_1^{-1}A_1)^{-1}A_1'C_1^{-1}Y \quad ,$$

and the prior mean

$$A_2A_3\theta_3 \quad ,$$

with weights equal to the inverse of the corresponding dispersion matrices,

$$A_1' \, C_1^{-1}A_1$$

for the least squares values, and

$$C_2 + A_2C_3A_2'$$

for the prior distribution. They also considered the estimation problem with unknown covariance structure; i.e. $\{C_i\}$ unknown. Because of the integration difficulties they considered, as an estimator, the mode of the joint posterior distribution of the parameter of interest and the nuisance parameters, which include the dispersion matrices C_i .

Box and Tiao (2) considered the problem of estimating the variance components for some balanced designs. They obtained an approximate posterior distribution of a linear function of the variance components. Their procedure depends on obtaining the posterior distribution of the expected mean square in the analysis of variance procedure and they considered an improper prior distribution for the variance components. Their method is restrictive because numerical integration must be employed to norm the distributions and to compute any posterior moments.

CHAPTER III

POSTERIOR DISTRIBUTION FOR THE VARIANCE COMPONENTS

Some Distribution Theory

Consider a mixed linear model

$$y = x\theta + ub + e, \tag{3.1}$$

where y is $N \times 1$ random vector whose observed values comprise the data points; x is a $N \times p$ $(N > p)$ full rank known design matrix, θ is a $p \times 1$ vector of real unknown parameters called the fixed effects;

$$u = (u_1, u_2, \ldots, u_c) \quad , \quad c \geq 1 \quad ;$$

u_i is $N \times m_i$ full rank known design matrix;

$$b' = (b_1, b_2, \ldots, b_c') \quad ;$$

b_i is a $m_i \times 1$ random vector distributed as $N(\Phi, \tau_i I_{m_i})$, where Φ is a null vector and $\tau_i I_{m_i}$ is the precision matrix; e is $N \times 1$ error vector distributed as $N(\Phi, \tau I_N)$, where τI_N is the precision matrix. The parameter space is

$$\Omega = \{(\theta, \tau, \tau_1, \ldots, \tau_c): \theta \varepsilon R^p; \tau > 0; \tau_i > 0, 1 \leq i \leq c\} .$$

The variance components are:

$$\sigma^2 = \tau^{-1} ,$$

$$\sigma_i^2 = \tau_i^{-1} , \quad 1 \leq i \leq c$$

and the fixed effects are the elements of θ.

Considering Bayes theorem, that is multiplying the likelihood function

$$L(\theta, b, \tau , \rho/y) = p(y|b, \theta, \tau , \rho)p(b|\rho) ,$$

where

$$\rho = (\tau_1, \tau_2, \ldots , \tau_c) ,$$

by the prior densities $p_0(\theta)$, $p_0(\tau)$, and $p_0(\rho)$; assuming that θ, τ, and ρ are independent, the joint posterior density of θ, b, τ, and ρ is given by

$$p(\theta, b, \tau , \rho |y) \propto \tau^{\frac{N}{2}} \exp\{ - \frac{\tau}{2} (y - x\theta - ub)'(y - x\theta - ub)\}$$

$$\times \prod_{i=1}^{c} \tau_i^{\frac{m_i}{2}} \exp \{-\tfrac{1}{2}\tau_i b_i' b_i\} p_0(\theta)p_0(\tau)p_0(\rho) ,$$

$$(\theta, b, \tau , \rho) \in \Omega \qquad (3.2)$$

Completing the square on θ in the above joint density, and letting $p_0(\theta) = \text{constant} \quad \theta \in R^p$, (3.2) can be written as

$$p(\theta, b, \tau, \rho | y) \propto \tau^{\frac{N}{2}} |v|^{\frac{1}{2}} \exp\{-\tfrac{1}{2}b'vb\}$$

$$\times \exp\{\tfrac{1}{2}\tau[(y - ub)'\ x(x'x)^{-1}x'(y-ub) - z]\}$$

$$\times\ p(\theta | b, y)p_0(\tau)p_0(\rho) \tag{3.3}$$

$$(\theta, b, \tau, \rho) \varepsilon\ \Omega$$

where

$$v = \text{Diag}\{\tau_1 I_{m_1}, \tau_2 I_{m_2}, \ldots, \tau_c I_{m_c}\},$$
$$z = (y - ub)'\ (y - ub), \quad \text{and}$$

$p(\theta | b,y)$ is the conditional posterior distribution of θ given b which is normal with mean vector

$$\theta^* = (x'x)^{-1}x'(y - ub)$$

and variance covariance matrix $(\tau x'x)^{-1}$. Thus, the joint posterior density of $b, \tau,$ and ρ can be obtained by integrating the right hand side of (3.3) with respect to θ, which leads to

$$p(b, \tau, \rho | y) \propto \tau^{\frac{N-p}{2}} |v|^{\frac{1}{2}} \exp\{\tfrac{\tau}{2}[(y - x\hat{\theta})'u(v + A)^{-1}u'(y - x\hat{\theta}) - z]\}$$

$$\times \exp\{-\tfrac{1}{2}b'vb\}p_0(\tau)p_0(\rho) \tag{3.4}$$

$$\rho > 0,\ \tau > 0,\ b\ \varepsilon\ R^m$$

Now, by completing the square on b in (3.4), it can be written as

$$p(b, \tau, \rho | y) \propto \tau^{\frac{N-p}{2}} |v|^{\frac{1}{2}} \exp\{\tfrac{\tau^2}{2} (y - x\hat{\theta})u(v + A)^{-1}u'(y - x\hat{\theta})$$

$$- \tfrac{\tau}{2}(y - x\hat{\theta})'(y - x\hat{\theta})\}p(b | \tau, \rho, y)p_0(\tau)p_0(\rho) \tag{3.5}$$

where

$$\hat{\theta} = (x'x)^{-1}x'y \quad ,$$

$$\Lambda = \tau u'[I - x(x'x)^{-1}x']u \quad , \quad \text{and}$$

$p(b|\tau, v, y)$ is the conditional posterior distribution of b given τ, and v, which is normal with mean vector

$$b^{*} = \tau(v + A)^{-1}u'(y - x\hat{\theta}), \quad \text{and}$$

variance covariance matrix $(v + A)^{-1}$.

The joint posterior density of τ and ρ can be obtained by integrating the right hand side of (3.5) with respect to b, namely

$$p(\tau , \rho|y) \propto \frac{\tau^{\frac{N-p}{2}}|v|^{\frac{1}{2}}}{|v + A|^{\frac{1}{2}}} \exp\{\frac{\tau^2}{2} (y - x\hat{\theta})'u(v + A)^{-1}u'(y - x\hat{\theta})\}$$

$$\times \exp\{-\frac{\tau}{2} (y - x\hat{\theta})'(y - x\hat{\theta})\} \; p_0(\tau)p_0(\rho) \tag{3.6}$$

$$\tau > 0, \rho > 0$$

$$\propto p(\tau|y)p(\rho|\tau , y)$$

where $$p(\tau|y) = c(\tau) \exp\{-\frac{\tau}{2} (y - x\hat{\theta})'(y - x\hat{\theta})\} p_0(\tau), \tau > 0 \tag{3.7}$$

$$c(\tau) = \int_0^\infty p_0(\rho)\frac{|v|^{\frac{1}{2}}}{|v + A|^{\frac{1}{2}}} \exp\{\frac{\tau^2}{2}(y - x\hat{\theta})'u(v + A)^{-1}u'(y - x\hat{\theta})\} d\rho ,$$

and

$$p(\rho|\tau ,y) \propto \frac{|v|^{\frac{1}{2}}}{|v + A|^{\frac{1}{2}}} \exp\{\frac{\tau^2}{2} (y - x\hat{\theta})'u(v + A)^{-1}u'(y - x\hat{\theta})\}p_0(\rho).$$

$$\rho > 0 \tag{3.8}$$

Since the conditional posterior distribution of θ given τ and b is normal with mean vector

$$\hat{\theta} - (x'x)^{-1}x'ub,$$

and variance covariance matrix $(\tau x'x)^{-1}$, and the conditional posterior distribution of b given τ, and ρ is normal with mean vector $\tau(v + A)^{-1}u'(y - x\hat{\theta})$, and variance covariance matrix $(v + A)^{-1}$, then

$$\begin{aligned} E(\theta|\tau, \rho, y) &= E_{b|\tau,\rho,y} E(\theta|\tau, b, y) \\ &= \hat{\theta} - \tau(x'x)^{-1}x'u(v + A)^{-1}u'(y - x\hat{\theta}), \end{aligned} \tag{3.9}$$

and

$$\begin{aligned} v(\theta|\tau,\rho, y) &= E_{b|\tau,\rho,y}[v(\theta|\tau, b, y) + v_{v|\tau,\rho,y} E(\theta|\tau, b, y) \\ &= (\tau x'x)^{-1} + (x'x)^{-1}x'u(v + A)^{-1}u'x(x'x)^{-1} \end{aligned} \tag{3.10}$$

i.e., the conditional posterior distribution of θ given τ and ρ is normal with mean vector defined in (3.9) and variance covariance matrix given in (3.10).

In the above discussion, the matrix $(v + A)$ is a positive definite matrix due to the fact that the maxtrix v is positive definite and the matrix A is a positive semi-definite. Also, the quadratic form

$$(y - x\hat{\theta})'u'(v + A)^{-1}u'(y - x\hat{\theta})$$

can be computed without inverting the matrix $(v + A)$. That can be done using the following fact introduced by Searle (13):

$$x'p^{-1}x = 1 - \frac{|p - xx'|}{|p|}$$

$$= \frac{|p + xx'|}{|p|} - 1$$

for any vector x and positive definite matrix p.

There are certain practical difficulties in the above procedure:

1. The marginal posterior distribution of τ must be determined numerically because of the factor $c(\tau)$.
2. The conditional posterior mean of τ given ρ must be determined numerically.
3. The choice of the improper prior distribution of τ and ρ.

One way to make inferences about all the parameters is in the following sequential fashion:

1. Determine the posterior distribution of τ, namely (3.7), then
2. Find the conditional distribution of ρ given τ, namely (3.8).
3. Determine the conditional posterior distribution of θ given ρ and τ.

One way to avoid the difficulty of determining the factor $c(\tau)$ numerically is to first find the conditional mean of ρ given

$$\tau^{-1} = \sigma^2 = \frac{(y - x\hat{\theta})'(y - x\hat{\theta})}{N - p} \tag{3.11}$$

which assumes $c(\tau)$ = constant and $p_0(\tau) = \tau^{N - p}$. Then one uses the posterior mean of τ as the conditioning value of τ. Once this is achieved one can use the conditional mean of θ, namely (3.9), to estimate θ. The conditional posterior mean of ρ is substituted into the diagonal elements of v, and (3.11) is used as the conditional value of σ^2.

Another more profitable approach for this problem is to assume that the prior distribution of τ_i be gamma with parameters $\alpha_i (> 0)$ and $\beta_i (> 0)$; and that τ is also gamma with parameters $\alpha (> 0)$ and $\beta (> 0)$. Therefore the joint posterior density (3.2) can be written as

$$p(\tau, \rho, \theta, b \mid y) \propto \tau^{\frac{N+2\alpha}{2} - 1} \exp\{-\tau [\beta + \tfrac{1}{2}(y - x\theta - ub)'(y - x\theta - ub)]\}$$

$$\times \prod_{i=1}^{c} \tau_i^{\frac{m_i + 2\alpha_i}{2} - 1} \exp\{-\tau_i(\beta_i + \tfrac{1}{2} b_i' b_i)\}, \qquad (3.12)$$

$$\tau, \rho, \theta, b \in \Omega$$

The joint posterior density (3.12) can be written in the following way.

$$p(\tau, \rho, \theta, b \mid y) \propto \tau^{\frac{N+2\alpha}{2} - 1} \exp\{-\tau [\beta + \tfrac{1}{2}(y - x\theta - ub)'(y - x\theta - ub)]\}$$

$$\times \prod_{i=1}^{c} (\beta_i + \tfrac{1}{2} b_i' b_i)^{-\frac{m_i + 2\alpha_i}{2}} p(\tau_i / b_i, y) \qquad (3.13)$$

$$\tau, \rho, \theta, b \in \Omega$$

where $p(\tau_i / b_i, y)$ is the conditional posterior distribution of τ_i given b_i $(i = 1, 2, \ldots, c)$, which is gamma with parameters $\frac{1}{2}(m_i + 2\alpha_i)$ and $(\beta_i + \frac{1}{2} b_i' b_i)$. The joint posterior density of τ, θ, and b can be obtained by integrating the right hand side of (3.13) with respect to ρ. Thus, the joint posterior density of τ, θ, and b can be written as

$$p(\tau,\theta,\ b|y) \propto [\beta + \tfrac{1}{2}(y-x\theta-ub)'(y-x\theta-ub)]^{-\frac{N+2\alpha}{2}} \prod_{i=1}^{c} [\beta_i+\tfrac{1}{2}b_i'b_i]^{-\frac{m_i+2\alpha_i}{2}}$$

$$\times\ p(\tau|\theta,b,y) \qquad \tau,\theta,\ b\ \varepsilon\ \Omega \qquad (3.14)$$

where $p(\tau|\theta,b,y)$ is the conditional posterior distribution of τ given θ and b, which is gamma with parameters $\frac{1}{2}(N+2\alpha)$ and $[\beta + \frac{1}{2}(y - x\theta - ub)'(y - x\theta - ub)]$. Integrating (3.14) with respect to τ, the joint posterior density of b and θ can be written as

$$p(b,\theta|y) \propto [1 + \frac{(b-b^*)'u'Ru(b-b^*)}{2\beta+s}]^{-\frac{m+(N+2\alpha-m-p)}{2}} \prod_{i=1}^{c} [1+\frac{1}{2\beta_i}b_i'b_i]^{-\frac{m_i+2\alpha_i}{2}}$$

$$\times\ p(\theta|b,y), \qquad \theta\ \varepsilon\ R^p,\ b\ \varepsilon\ R^m, \qquad (3.15)$$

where $\theta^* = (x'x)^{-1}x'(y - ub)$,

$R = I - x(x'x)^{-1}x'$,

$s = y'R[I - u(u'Ru)^{-}u']Ry,$

$b^* = (u'Ru)^{-}u'Ry$,

and $p(\theta|b,y)$ is the conditional posterior distribution of θ given b, which is a p-variate t distribution with $\frac{1}{2}(N+2\alpha-p)$ degrees of freedom, location vector θ^* and precision matrix

$$\frac{(N+2\alpha-p)(x'x)}{2\beta+(b-b^*)'u'Ru(b-b^*)+s} .$$

Integrating (3.15) with respect to θ, the marginal posterior distribution of b is as follows

$$p(b|y) \propto \left[1 + \frac{(b-b^*)'u'Ru(b-b^*)}{2\beta+s}\right]^{-\frac{m+(N+2\alpha-m-p)}{2}}$$

$$\times \prod_{i=1}^{c} \left[1 + \frac{1}{2\beta_i} b_i' b_i\right]^{-\frac{m_i+2\alpha_i}{2}} \quad . \qquad b \in R^m \quad (3.16)$$

In order to compute the conditional posterior means of τ, $\tau_i (i=1, \ldots, c)$, and the fixed effects θ, it is required to have an estimate for the random vector b. Since the marginal posterior distribution of b, given in (3.16), is not easy to handle in order to compute the posterior mean of random vector b, then it will be more convenient to consider b as a constant unknown parameter vector. That can be done considering the model (3.1) after multiplying both sides by the matrix R; namely,

$$Ry = Rub + Re \quad .$$

Then, the least square estimator of b, namely

$$b^* = (u'Ru)^- u'Ry \quad , \qquad (3.17)$$

will be considered as a conditioning value of b. Although b^* is a biased estimator of b, the variance covariance matrix of b^* is

$$\mathrm{Var}(b^*) = (u'Ru)^- \sigma^2 \quad .$$

The proposed approach to estimating τ and ρ can be summarized in the following sequential fashion:

1. Determine the estimator of b, namely,

$$b^* = (u'Ru)^- u'Ry \quad ,$$

2. determine the mean vector of θ conditional on $b=b^*$, namely,

$$\theta^* = (x'x)^{-1} x'(y-ub^*) \quad ,$$

3. determine the expected value of τ or σ^2, conditioned on $b=b^*$ and $\theta=\theta^*$, namely,

$$E(\tau | \theta^*, b^*) = \frac{N+2\alpha}{2\beta+(y-x\theta^*-ub^*)'(y-x\theta^*-ub^*)} \quad , \tag{3.18}$$

or

$$E(\sigma^2 | \theta^*, b^*) = \frac{2\beta+(y-x\theta^*-ub^*)'(y-x\theta^*-ub^*)}{N+2\alpha-2} \quad .$$

4. determine the expected value of τ_i or σ_i^2 $(i = 1, 2, \ldots, c)$, conditional on $b_i = b_i^*$ (b_i^* is the ith subvector of dimension m_i in b^*), namely

$$E(\tau_i | b_i^*) = \frac{m_i + 2\alpha_i}{2\beta_i + b_i^{*\prime} b_i^*} \quad , \tag{3.19}$$

or

$$E(\sigma_i^2 | b_i^*) = \frac{2\beta_i + b_i^{*\prime} b_i^*}{m_i + 2\alpha_i - 2} \quad .$$

The remainder of this chapter will concern some balanced layouts. The main object of the above approach was estimating the vector b which depends on the generalized inverse of the matrix $u'Ru$. The generalized inverse of a singular matrix z will be considered to be that matrix z^- such that

1. zz^- is symmetric,
2. z^-z is symmetric,
3. $z^-zz^- = z^-$, and
4. $zz^-z = z$.

One-way Random Model

For this particular model, using the notation of (3.1), pages 11 and 12, $p = 1$, $c = 1$, $m_1 = a$, and $N = an$, where a is the number of observations in each group. The matrix $u'Ru$ has the structure

$$nI_a - \frac{n}{a} J_a \quad ,$$

where I_a is the identity matrix of order a , and J_a is axa matrix of ones. Then,

$$(u'Ru)^- = \frac{1}{n} (I_a - \frac{1}{a} J_a) \quad .$$

The vector b is estimated by

$$b^* = \begin{bmatrix} \bar{y}_{1\cdot} - \bar{y}_{\cdot\cdot} \\ \bar{y}_{2\cdot} - \bar{y}_{\cdot\cdot} \\ \vdots \\ \bar{y}_{a\cdot} - \bar{y}_{\cdot\cdot} \end{bmatrix} \quad ,$$

where $y_{i\cdot}$ $(i = 1, 2, \ldots, a)$ is the treatment means, and $\bar{y}_{\cdot\cdot}$ is the overall mean. The conditional posterior mean of θ (given $b = b^*$) is given by

$$\theta^* = \bar{y}_{\cdot\cdot} \ .$$

One more quantity which has special importance in computing the conditional posterior mean of τ (given $b = b^*$ and $\theta = \theta^*$) is

$$(y - x\theta^* - ub^*)'(y - x\theta^* - ub^*) = \sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \bar{y}_{i\cdot})^2 \ ,$$

where y_{ij} is the j^{th} observation in the i^{th} treatment.

Two-fold Nested Random Model

Consider the first treatment with a levels, the second treatment with b levels in each of the a levels of the first treatment, and n observations in each treatment combination. Then using the notation of (3.1), the model takes the form $y_{ijk} = \theta+\delta_i+\gamma_{ij}+e_{ijk}$, $i = 1,2,\ldots a$, $j = 1,2,\ldots,b$, $k = 1,2,\ldots,n$; therefore $p=1$, $c=2$, $m_1=a$, $m_2=b$, and N-abn. Now the matrix U'RU has the structure

$$n \begin{bmatrix} bI_a - \frac{b}{a} J_a & A - \frac{1}{a} j_a j'_{ab} \\ A' - \frac{1}{a} j_{ab} j'_a & I_{ab} - \frac{1}{ab} J_{ab} \end{bmatrix}$$

where I and J as defined before, and j is a x 1 vector of ones.

Then

$$(u'Ru)^{-} = \frac{1}{n(b+1)^2} \begin{bmatrix} b(I_a - \frac{1}{a}J_a) & A - \frac{1}{a} j_a j'_{ab} \\ A - \frac{1}{a} j_{ab} j'_a & (b+1)^2 I_{ab} - (b+2)A'A - \frac{1}{ab} J_{ab} \end{bmatrix}$$

where A is $axab$ matrix of the form

$$\begin{bmatrix} j'_b & & & & \\ & j'_b & & \Phi & \\ & & \cdot & & \\ & & & \cdot & \\ \Phi & & & \cdot & j'_b \end{bmatrix} .$$

The following quantities are those which one needs in computing the conditional posterior means.

$$b_1^{*\prime} b_1^{*} = \frac{b^2}{(b+1)^2} \sum_{i=1}^{a} (\bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot\cdot\cdot})^2$$

$$b_2^{*\prime} b_2^{*} = \sum_{i=1}^{a} \sum_{j=1}^{b} (\bar{y}_{ij\cdot} - \frac{b}{b+1} \bar{y}_{i\cdot\cdot} - \frac{1}{b+1} \bar{y}_{\cdot\cdot\cdot})^2 ,$$

$$\theta^* = \bar{y}_{\cdot\cdot\cdot} \quad , \quad \text{and}$$

$$(y - x\theta^* - ub^*)'(y - x\theta^* - ub^*) = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{n} (y_{ijk} - \bar{y}_{ij\cdot})^2$$

Two-Way Random Model (with Interaction)

Considering the first random factor of r levels and the second random factor at t levels. Then, using the notation of (3.1), the model takes the form

$$y_{ijk} = \Theta + \alpha_i + \beta_j + \gamma_{ij} + e_{ijk} ,$$

$i = 1, 2, \ldots, r$, $j = 1, 2, \ldots, t$, $k = 1, 2, \ldots, n$; therefore, $p = 1$, $c = 3$, $m_1 = r$, $m_2 = t$, $m_3 = rt$, and $N = rtn$, where n is the number of observations in each of the rt treatment combinations. The structure of the matrix $u'Ru$ is of the form

$$\begin{bmatrix} tn(I_r - \frac{1}{r} J_r) & 0 & n(A - \frac{1}{r} j_r j_{rt}') \\ 0 & rn(I_t - \frac{1}{t} J_t) & n(B - j_t j_{rt}') \\ n(A' - \frac{1}{r} j_{rt} j_r') & n(B' - \frac{1}{t} j_{rt} j_t') & n(I_{rt} - \frac{1}{rt} J_{rt}) \end{bmatrix}$$

where A is $r \mathrm{x} rt$ matrix of the form

$$\begin{bmatrix} j_t' & & & & \Phi \\ & j_t' & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ \Phi & & & & j_t' \end{bmatrix} , \qquad \text{and}$$

B is txrt matrix of the form

$$[I_t \ \ I_t \ \cdots \ I_t] \quad .$$

The generalized inverse is found to be

$$(u'Ru)^{-} = \begin{bmatrix} \frac{t}{n(t+1)^2}(I_r - \frac{1}{r} J_r) & 0 & \frac{1}{n(t+1)^2}(A - \frac{1}{r} j_r j_{rt}') \\ 0 & \frac{r}{n(r+1)^2}(I_t - \frac{1}{t} J_t) & \frac{1}{n(r+1)^2}(B - \frac{1}{t} j_t j_{rt}') \\ \frac{1}{n(t+1)^2}(A' - \frac{1}{r} j_{rt} j_r') & \frac{1}{n(r+1)^2}(B' - \frac{1}{t} j_{rt} j_t') & D \end{bmatrix}$$

where

$$D = \frac{1}{n} I_{rt} - \frac{t+2}{n(t+1)^2} A'A - \frac{r+2}{n(r+1)^2} B'B + \left[\frac{1}{nr(t+1)^2} + \frac{1}{nt(r+1)^2} + \frac{rt-1}{nr(r+1)(t+1)} \right] J_{rt} \quad .$$

The quantities of interest in this case are

$$b_1^{*\prime} b_1^{*} = \frac{t^2}{(t+1)^2} \sum_{i=1}^{r} (\bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot\cdot\cdot})^2 \quad ,$$

$$b_2^{*\prime} b_2^{*} = \frac{r^2}{(r+1)^2} \sum_{j=1}^{t} (\bar{y}_{\cdot j\cdot} - \bar{y}_{\cdot\cdot\cdot})^2 \quad ,$$

$$b_3^{*\prime} b_3^* = \sum_{i=1}^{r} \sum_{j=1}^{t} (\bar{y}_{ij\cdot} - \frac{t}{t+1} \bar{y}_{i\cdot\cdot} - \frac{r}{r+1} \bar{y}_{\cdot j\cdot} + \frac{rt-1}{(r+1)(t+1)} \bar{y}_{\cdot\cdot\cdot})^2 ,$$

$$\theta^* = \bar{y}_{\cdot\cdot\cdot} , \quad \text{and}$$

$$(y - x\theta^* - ub^*)'(y - x\theta^* - ub^*) = \sum_{i=1}^{r} \sum_{j=1}^{t} \sum_{k=1}^{n} (y_{ijk} - \bar{y}_{ij\cdot})^2 .$$

Two-Way Random Model (Without Interaction)

Assuming that the first random factor has r levels, and the second random factor has t levels, then using the notation of (3.1), the model takes the form

$$y_{ijk} = \theta + \alpha_i + \gamma_j + e_{ijk} ,$$

$i = 1, 2, \ldots, a$, $j = 1, 2, \ldots, b$, $k = 1, 2, \ldots, n$; therefore, $p = 1$, $m_1 = r$, $m_2 = t$, $c = 2$, and $N = rtn$ where n is the number of observations in each of the rt treatment combinations. The structure of the matrix $u'Ru$ has the following symmetric structure,

$$u'Ru = \begin{bmatrix} tn(I_r - \frac{1}{r} J_r) & 0 \\ 0 & rn(I_t - \frac{1}{t} J_t) \end{bmatrix} .$$

Thus,

$$(u'Ru)^- = \begin{bmatrix} \frac{1}{tn} (I_r - \frac{1}{r} J_r) & 0 \\ 0 & \frac{1}{rn}(I_t - \frac{1}{t} J_t) \end{bmatrix} ,$$

$$b_1^{*\prime} b_1^* = \sum_{i=1}^{r} (\bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot\cdot\cdot})^2 \quad ,$$

$$b_2^{*\prime} b_2^* = \sum_{j=1}^{t} (\bar{y}_{\cdot j\cdot} - \bar{y}_{\cdot\cdot\cdot})^2 \quad ,$$

$$\theta^* = \bar{y}_{\cdot\cdot\cdot} \quad , \text{ and}$$

$$(y-x\theta^*-ub^*)'(y-x\theta^*-ub^*) = \sum_{i=1}^{r} \sum_{j=1}^{t} \sum_{k=1}^{n} (y_{ijk}-\bar{y}_{i\cdot\cdot}-\bar{y}_{\cdot j\cdot}+\bar{y}_{\cdot\cdot\cdot})^2$$

Two-Way Mixed Model (with Interaction)

Consider the fixed effect with p levels, the random effects with a levels and n observations for each of the ap treatment combinations. Then using the notation of (3.1), the model takes the form $y_{ijk} = \Theta_i + \alpha_j + \gamma_{ij} + e_{ijk}$, $i = 1, 2, \ldots, p$, $j = 1, 2, \ldots, a$, $k = 1, 2, \ldots, n$; therefore, $m_1 = a$, $c = 1$, and $N = apn$. Also,

$$u'Ru = \begin{bmatrix} np(I_a - \frac{1}{a} J_a) & n(A - \frac{1}{a} j_a j_{ap}') \\ & \\ n(A' - \frac{1}{a} j_{ap} j_a') & n(I_{ap} - \frac{1}{a} B'B) \end{bmatrix}$$

where B is $pxap$ matrix of the form

$$\begin{bmatrix} j_a' & & & \\ & j_a' & & \\ & & \ddots & \\ & & & j_a' \end{bmatrix} \quad , \text{ and}$$

A is axap matrix of the form

$$[I_a \ \ I_a \cdots I_a] \quad .$$

Thus,

$$(u'Ru)^{-} = \begin{bmatrix} \frac{p}{n(p+1)^2}(I_a - \frac{1}{a} J_a) & \frac{1}{n(p+1)^2}(A - \frac{1}{a} j_a j_{ap}') \\ \frac{1}{n(p+1)^2}(A' - \frac{1}{a} j_{ap} j_a') & \frac{1}{n}(I_{ap} - \frac{1}{a} B'B) - \frac{p+2}{N(p+1)^2}(A'A - \frac{1}{a} J_{ap}) \end{bmatrix} ,$$

$$b_1^{*\prime} b_1^* = \sum_{j=1}^{a} (\bar{y}_{\cdot j \cdot} - \bar{y}_{\cdots})^2 \quad ,$$

$$\theta^* = \begin{bmatrix} \bar{y}_{1\cdot\cdot} \\ \bar{y}_{2\cdot\cdot} \\ \vdots \\ \bar{y}_{p\cdot\cdot} \end{bmatrix} \quad , \text{ and}$$

$$(y - x\theta^* - ub^*)'(y - x\theta^* - ub^*) = \sum_{i=1}^{p} \sum_{j=1}^{a} \sum_{k=1}^{n} (y_{ijk} - \bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot j \cdot} + \bar{y}_{\cdots})^2 \quad .$$

Two-Way Mixed Model (Without Interaction)

Consider the fixed effect with p levels, the random effects with a levels and n observations in each ap treatment combination. Then, using the notation of (3.1), the model takes the form

$y_{ijk} = \theta_i + \alpha_j + e_{ijk}$, $i = 1, 2, \ldots, p$, $j = 1, 2, \ldots, a$,

$k = 1, 2, \ldots, n$; therefore, $c = 1$, $m_1 = a$, and $N = apn$. Also,

$$u'Ru = np(I_a - \frac{1}{a} J_a) \quad .$$

Thus,

$$(u'Ru)^- = \frac{1}{np} (I_a - \frac{1}{a} J_a) \quad ,$$

$$b^{*\prime}b^* = \sum_{j=1}^{a} (\bar{y}_{\cdot j \cdot} - \bar{y}_{\cdots})^2 ,$$

$$\theta^* = \begin{bmatrix} \bar{y}_{1\cdot\cdot} \\ \bar{y}_{2\cdot\cdot} \\ \cdot \\ \cdot \\ \cdot \\ \bar{y}_{p\cdot\cdot} \end{bmatrix} \quad , \text{ and}$$

$$(y-x\theta^*-ub^*)'(y-x\theta^*-ub^*) = \sum_{i=1}^{p} \sum_{j=1}^{a} \sum_{k=1}^{n} (y_{ijk} - \bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot j \cdot} + \bar{y}_{\cdots})^2 \quad .$$

In the case of having unbalanced design, the problem of computing the generalized inverse of the matrix $u'Ru$ will not be a simple one. However, in one-way layout with unbalanced data, the problem is less complicated than other types of design. Consider a levels of the treatment effects each has n_i $(i = 1, 2, \ldots, a)$ observations. Then,

$$p = 1 ,$$

$$m_1 = a , \quad \text{and}$$

$$N = \sum_{i=1}^{a} n_i .$$

Also,

$$u'Ru = \begin{bmatrix} n_1(1 - \frac{n_1}{N}) & -\frac{n_1 n_2}{N} & \cdots & -\frac{n_1 n_a}{N} \\ -\frac{n_1 n_a}{N} & n_2(1 - \frac{n_2}{N}) & \cdots & \frac{n_2 n_a}{N} \\ \vdots & \vdots & & \vdots \\ -\frac{n_1 n_a}{N} & -\frac{n_2 n_a}{N} & \cdots & n_a(1 - \frac{n_a}{N}) \end{bmatrix} .$$

Thus,

$$(u'Ru)^{-} = \frac{1}{N} \begin{bmatrix} \frac{N-n_1}{n_1} & -1 & -1 & \cdots & -1 \\ -1 & \frac{N-n_2}{n_2} & -1 & \cdots & -1 \\ \vdots & \vdots & \ddots & & \vdots \\ -1 & -1 & -1 & \cdots & \frac{N-n_a}{n_a} \end{bmatrix} ,$$

$$b^{*\prime}b^{*} = \sum_{i=1}^{a} (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot})^2 ,$$

$$\theta^{*} = \bar{y}_{\cdot\cdot} , \quad \text{and}$$

$$(y-x\theta^*-ub^*)'(y-x\theta^*-ub^*) = \sum_{i=1}^{a} \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i\cdot})^2$$

In the appendix a description for a computer program using a SAS routine is given, by which one can compute any of these quantities required for the result of Chapter III.

Example:

Box and Tiao (2) generated a set of data for a one-way random model design. The within groups variance component σ^2, and the between groups variance component σ_1^2 have been estimated using their analysis as well as the analysis introduced in this chapter. They found that (12.133, 0.0) is a joint model estimate of (σ^2, σ_1^2), also they found that the marginal posterior means of σ^2 and σ_1^2 are 14.95 and 3.0, respectively.

Equations (3.18) and (3.19) shows that

$$E(\sigma^2 | \theta^*, b^*) = 12.8108,$$

and

$$E(\sigma_1^2 | b^*) = 2.0841 \quad .$$

The analysis of variance procedure shows that

$$\hat{\sigma}^2 = 14.9459 \quad ,$$

and

$$\hat{\sigma}_1^2 = -1.3219 \quad ,$$

where $\hat{\sigma}^2$ and $\hat{\sigma}_1^2$ are estimates of the within groups and between groups variance components.

The true values were

$$\sigma^2 = 16 \quad ,$$

and

$$\sigma_1^2 = 4 \quad .$$

CHAPTER IV

SUMMARY

The main objective of this thesis is to develop a Bayesian methodology, which produces point estimators for the parameters of mixed linear models. This methodology is based on a new theoretical analysis which finds the exact conditional posterior distribution of the variance components, given the random and fixed effects, and the posterior distribution of the random and fixed effects.

Instead of employing the marginal distribution of the variance components, but using their conditional distribution, one is able to provide inferences for the variance components from independent gamma distributions. It has been shown that the conditional posterior distribution of $\tau\,(=\bar{\sigma}^{2})$ and ρ, where $\rho' = (\tau_1, \tau_2, \ldots, \tau_c)$, where $\tau_i = \sigma_i^{-2}$, given θ and b, is that of $c+1$ independent gamma variables. Also it is shown that the conditional posterior distribution of θ given b is a general t with location vector $(x'x)^{-1}x'(y-ub)$ and that the marginal posterior mode of b is approximately $b^* = (uRu)^{-}u'Ry$.

All the developments in Chapter III assumes that $\theta, \tau,$ and ρ are independent and that a priori, θ has a constant density, τ has a gamma density and $\tau_1, \tau_2, \ldots, \tau_c$ are independent and have gamma distributions. The conditional posterior means of τ and τ_i given θ and b are

$$E(\tau \mid \theta, b) = (N + 2\alpha)[2\beta + (y-x\theta-ub)'(y-x\theta-ub)]^{-1} ,$$

and

$$E(\tau_i \mid \theta, b) = \frac{m_i + 2\alpha_i}{2\beta_i + b_i' b_i} .$$

The error variance τ^{-1} and variance components τ_i^{-1} are estimated from the above conditional means by conditioning with

$$\theta = \theta^* = (x'x)^{-1}x'(y-ub) ,$$

and

$$b = b^* = (u'Ru)^{-}u'Ry .$$

These estimators are algebraically derived for some special random and mixed models, including the one-way, two-fold nested, two-way crossed random, and two-way crossed mixed models.

The proposed estimators are just one of many that could have been considered and no attempt has been made to justify their use. If a square error loss function is appropriate, then these estimators are approximately Bayes estimators.

The principal goal of a Bayesian analysis is to know the joint posterior distribution of all the parameters in the model and this dissertation has made a substantial contribution in that direction.

The goal of additional research will be to find and completely determine the marginal posterior distribution of the variance components, error variance, and fixed effects. Also, to find convenient algebraic formulas for the moments (means and variances) of these parameters is an essential component of a satisfactory solution.

From the non-Bayesian viewpoint, further investigation into the sampling properties of the conditional posterior means of the variance components could be attempted. An interesting question is what values of α, β, α_i and β_i , $i = 1, 2, \ldots, c$ produce minimum mean square estimators, and how do these compare to some of the non-Bayesian estimators such as maximum-likelihood, MIVQUE, and Henderson's techniques?

Another possibility for further work is to generalize the results of this dissertation to multivariate mixed models; i.e., those which include multiple measurements on each sampling unit and to models which contain correlated random factors. Multivariate mixed models are quite useful in quantitative genetics, where one is interested in variance and covariance components. It appears that these generalizations are quite feasible.

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APPENDIX

The following computer routine is designed according to SAS User's Guide (1976). The inputs requred are: the vector y, the number of variance components c, the m_i values ($i = 1, 2, \ldots, c$), the design matrix x, and the design matrix u. The out-put contains the vectors b^*, θ^*, and the quantities $b_i^{*\prime} b_i^*$ ($i = 1, 2, \ldots, c$) and $(y - x\theta^* - ub^*)'(y - x\theta^* - ub^*)$.

```
PROC MATRIX;
Y    = (The data vector in the form  y11/y12/...) ;
IC   = (The value of  c);
MB   = (m1/m2/.../mc) ;
X    = (The design matrix  x  written row at a time, and a "/" separating
        the rows) ;
U   = (The design matrix  u  written in the same format as  X) ;
XT   =  X' ;
XTX   =  XT * X  ;
XTX   =  INV(XTX) ;
N   =  NROW(X) ;
R   =  I(N)  - X * XTX * XT  ;
UTR   =  U' * R ;
UTRU   =  UTR * U ;
BHAT   =  GINV(UTRU) * UTR * Y  ;
FREE  UTR  ;
PRINT  BHAT ;
UBHAT   =  U * BHAT  ;
FREE U  ;
THETA   =  XTX * XT * (Y  - UBHAT)  ;
PRINT THETA  ;
RESID   =  Y - X * THETA  - UBHAT  ;
FREE THETA  ;
RES   =  RESID' * RESID  ;
FREE RESID  ;
PRINT RES  ;
MI   =  0  ;
```

```
BB  =  j(IC, 1, 0)  ;
I  =  0  ;
INC  =  0  ;
     LOOP1      :  I  =  I + 1  ;
                  MI  =  MI + MB(I + 1)  ;
                   j  =  INC  ;
     LOOP2      :  j  =  j + 1  ;
                  BB(I, 1)  =  BB(I + 1) + BHAT(j,1) * BHAT(j,1)  ;
                  IF  j < MI  THEN GO TO LOOP2  ;
                  INC  =  INC + MI  ;
                  IF  I < IC  THEN GO TO LOOP1  ;
PRINT BB  ;
```

*The elements of BB are the values of $b_i^{*\prime} b_i^*$ *

*The vector THETA equivalent to θ^* *

*The value of RES equivalent to $(y-x\theta^*-ub^*)'(y-x\theta^*-ub^*)$ *

*The vector BHAT equivalent to b^* *

VITA

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