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Two-Stage Analysis Based on a Mixed Model: Large-Sample Asymptotic Theory and Small-Sample Simulation Results

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SUMMARY

A two-stage analysis for the mixed model in which variance components due to the random effects are estimated and used to compute generalized least squares estimates of fixed effects is developed. Large-sample theory is used to establish asymptotic properties. An approximate t test that can be used to test linear contrasts among fixed effects is discussed. Two modest simulations, based on a model for a grazing trial (Burns, Harvey, and Giesbrecht, 1981, *Proceedings of 14th International Grassland Conference*, J. A. Smith and V. W. Hays (eds), 497–500, Boulder, Colorado: Westview Press; Burns et al., 1983, *Agronomy Journal* **75,** 865–871) are used to show that the asymptotic results are reasonable for small samples.

1. Introduction

Practicing statisticians often encounter problems in which the appropriate linear model includes fixed effects and random effects in addition to the usual residual error term. The fixed effects are of primary interest and the random effects represent sources of error. Experiments employing incomplete block designs with blocks random and split-plot experiments are examples that lead to models of this form. In both of these cases the loss of some observations causes a loss of balance and complicates the analysis. Alternatively, one encounters the same problem in field experiments repeated over a number of years, in which some treatments are shifted from field to field (assumed random) while other fields retain the same treatments over a number of years. A grazing trial involving 19 fields and 12 treatments over a period of 6 years motivated this study and provides the basis for a simulation study.

Formally, the linear model suitable for data from such unbalanced mixed model experiments can be written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{U}_1\mathbf{e}_1 + \cdots + \mathbf{U}_k\mathbf{e}_k \tag{1.1}$$

where

$\mathbf{Y}$ is the vector of n observations;
$\mathbf{X}$ is an $(n \times p)$ matrix of fixed constants of rank p;
$\boldsymbol{\beta}$ is a vector of p unknown parameters;
$\mathbf{U}_i$ is an $(n \times m_i)$ matrix of known constants;
$\mathbf{e}_i$ is a vector of m_i independent random errors with mean 0 and variance σ_i^2.

Key words: Estimation and testing in mixed models; Generalized least squares; Mixed model; Two-stage analysis; Variance components.

Frequently, though not necessarily, $\mathbf{U}_k$ will be the identity matrix. It follows that $\mathbf{E}(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta}$ and $\mathbf{V}(\mathbf{Y}) = \sum \mathbf{U}_i \mathbf{U}_i' \sigma_i^2 = \mathbf{V}$ is a positive definite $(n \times n)$ covariance matrix. Also, it is well known that the best linear unbiased estimate for $\boldsymbol{\beta}$ is the generalized least squares estimator

$$\tilde{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{Y} \tag{1.2}$$

with covariance matrix

$$\operatorname{cov}(\tilde{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}. \tag{1.3}$$

The practitioner who intends to use these results quickly encounters several problems. First, in the general unbalanced case both $\tilde{\boldsymbol{\beta}}$ and $\operatorname{cov}(\tilde{\boldsymbol{\beta}})$ depend on $\{\sigma_i^2\}$. Typically these parameters are unknown and must be estimated from the data. Second, even if good estimates $\{\hat{\sigma}_i^2\}$ are available, the size of $\mathbf{V}$ makes the task of computing $\mathbf{V}^{-1}$ formidable. Finally, the user who has surmounted these difficulties finds that the literature gives only asymptotic large-sample properties for the estimators. The object of this note is to present a possible solution to the computational difficulties for problems of modest size and a simulation study to illustrate the small-sample properties.

2. Previous Approaches

A common method for handling model (1.1) is to assume away the problem, i.e., proceed as though $\mathbf{V} = \sigma^2\mathbf{I}$ and use ordinary least squares. It is well known that the resulting estimates, $\hat{\boldsymbol{\beta}}_{\mathrm{LS}}$, are unbiased. Also, an unbiased estimate of $\operatorname{cov}(\hat{\boldsymbol{\beta}}_{\mathrm{LS}})$ can be obtained by using unbiased $\{\hat{\sigma}_i^2\}$ and computing $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\hat{\mathbf{V}}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$. When the random effects define an error structure of the nested type, then Fuller and Battese (1973) show how the solution $\tilde{\boldsymbol{\beta}}$ can be obtained without having to invert the $n \times n$ matrix. They propose to use the "fitting-of-constants" estimators (Searle, 1971, p. 443) for the variance components and then replace $\mathbf{V}$ by $\sum \mathbf{U}_i' \mathbf{U}_i \hat{\sigma}_i^2$. They establish conditions under which their proposed generalized least squares estimator is unbiased and asymptotically equivalent to the true generalized least squares estimator. Rao and Subrahmaniam (1971) and Rao (1973) investigate the problems of combining k independent means with unequal variances and estimating regression coefficients in a linear regression model with heteroscedastic variances. They show that using minimum norm quadratic unbiased estimates (MINQUE) of the variance components in a weighted least squares estimation can lead to considerable gain in efficiency even with relatively small samples.

Hemmerle and Hartley (1973) assume that the $\mathbf{e}_i \sim \mathrm{N}_{m_i}(\mathbf{0}, \mathbf{I}\sigma_i^2)$ in (1.1) and apply the W-transformation to obtain maximum likelihood estimates for $\boldsymbol{\beta}$. This method allows quite general models and provides the asymptotic covariance matrix of the vector of estimates. Corbeil and Searle (1976) provide a general method, again based on the W-transformation but using the restricted or modified maximum likelihood methodology of Patterson and Thompson (1971). The Corbeil and Searle method allows a mixed model and has the advantage that when applied to balanced cases it leads to the same answers as the conventional analysis of variance. A unification in the general mixed analysis of variance model is given by Jennrich and Sampson (1976). Using the basic W-transformation, they develop a Newton–Raphson algorithm and a Fisher scoring algorithm, both distinct from the hybrid between a generalized least squares and the Newton–Raphson algorithm of Hemmerle and Hartley.

3. The Procedure

The method of analysis proposed in this paper consists of two phases, one to estimate the variance components and a second to estimate the fixed effects using generalized least squares based on an estimated covariance matrix $\hat{\mathbf{V}}$ obtained via the $\{\hat{\sigma}_i^2\}$. The first phase again consists of two steps: an initial MINQUE (Rao, 1969) step followed by a MIVQUE (Rao, 1971) step using estimates obtained in the first step as "prior" values. Note that since these "prior" values are data-dependent, the proof of unbiasedness no longer holds. Since neither MINQUE nor MIVQUE gives any assurance that the estimates produced will be nonnegative, both steps require appropriate checks. Note also that if one assumes normality and repeats the MIVQUE steps until convergence (with proper restrictions on negative values) then one has restricted maximum likelihood (REML) estimates. In practice, convergence tends to be very rapid and the values proposed can be interpreted as equivalent to REML estimates. A Monte Carlo study by Swallow and Monahan (1984) using an unbalanced among and within model indicates that iterating to convergence is of limited value.

A point to notice in the computation is that the matrix $\mathbf{X}'\tilde{\mathbf{V}}^{-1}\mathbf{X}$ (and the column $\mathbf{X}'\tilde{\mathbf{V}}^{-1}\mathbf{Y}$), where

$$\tilde{\mathbf{V}} = \alpha_1\mathbf{U}_1\mathbf{U}_1' + \alpha_2\mathbf{U}_2\mathbf{U}_2' + \cdots + \alpha_k\mathbf{U}_k\mathbf{U}_k'$$

can be obtained by repeated use of the formula

$$\mathbf{X}'(\alpha_r\mathbf{U}_r\mathbf{U}_r' + \mathbf{V}_r)^{-1}\mathbf{X} = \mathbf{X}'\mathbf{V}_r^{-1}\mathbf{X} - \alpha_r\mathbf{X}'\mathbf{V}_r^{-1}\mathbf{U}_r(\mathbf{I}_r + \alpha_r\mathbf{U}_r'\mathbf{V}_r^{-1}\mathbf{U}_r)^{-1}\mathbf{U}_r'\mathbf{V}_r^{-1}\mathbf{X},$$

where $\mathbf{V}_r = \sum_{l=r+1}^{k} \alpha_l\mathbf{U}_l\mathbf{U}_l'$ and $\mathbf{I}_r$ is the $m_r \times m_r$ identity matrix. For many problems the computational task now is manageable, with the largest matrix to be inverted being $\max(m_i) \times \max(m_i)$. Other computational strategies (for example, Patterson and Thompson, 1974) are possible and will yield equivalent results. Very large problems will require more sophisticated programming in order to accommodate the large matrices being manipulated (Giesbrecht, 1983).

If $\{\hat{\sigma}_i^2\}$ represent the variance component estimates and $\hat{\mathbf{V}} = \sum \hat{\sigma}_i^2\mathbf{U}_i\mathbf{U}_i'$, then the estimates of the fixed effects are obtained as

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{Y}. \tag{3.1}$$

Note that without special checks to eliminate unacceptable values, MIVQUE does not guarantee that $\hat{\mathbf{V}}$ as computed above will be nonsingular. Consequently, without these special checks, the Kackiwani (1968) and Kackar and Harville (1981) result, i.e., unbiased fixed effects, does not follow directly. Replacing negative estimates of σ_l^2 with zeros for $l = 1, \ldots, k-1$ and negative estimates of σ_k^2 with δ, where δ is a small positive value, is sufficient to avoid difficulties [see Giesbrecht (1983)]. An alternative is to use the "fitting-of-constants" estimate of σ_k^2.

As shown by Fuller and Battese (1973), an approximate covariance matrix for the estimates is $(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}$. It follows that the standard errors of the elements of $\hat{\boldsymbol{\beta}}$ are given by $S_1, \ldots, S_p$, the positive square roots of the elements on the main diagonal of the covariance matrix. Approximate tests of hypotheses and confidence intervals can be made using the t distribution. Satterthwaite's (1941) approximation is used to provide the approximate degrees of freedom:

$$\mathrm{df}_i \approx 2S_i^2/[\text{approx. var}(S_i^2)]. \tag{3.2}$$

In general, one wants contrasts of the form $\boldsymbol{\lambda}'\hat{\boldsymbol{\beta}}$ to estimate $\boldsymbol{\lambda}'\boldsymbol{\beta}$. This contrast has approximate variance $\boldsymbol{\lambda}'(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\boldsymbol{\lambda}$. The degrees of freedom for this contrast must be approximated. In particular, using a Taylor series approximation, we have

$$\begin{aligned} &\mathrm{var}[\boldsymbol{\lambda}'(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\boldsymbol{\lambda}] \\ &\quad \approx \sum_{i,j}^{k} \mathrm{cov}(\hat{\sigma}_i^2, \hat{\sigma}_j^2)(\boldsymbol{\lambda}'\mathbf{P}\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{U}_i\mathbf{U}_i'\hat{\mathbf{V}}^{-1}\mathbf{X}\mathbf{P}\boldsymbol{\lambda})(\boldsymbol{\lambda}'\mathbf{P}\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{U}_j\mathbf{U}_j'\hat{\mathbf{V}}^{-1}\mathbf{X}\mathbf{P}\boldsymbol{\lambda}), \end{aligned} \tag{3.3}$$

where $\mathbf{P} = (\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}$ and a rough approximation to the covariance matrix of $\{\hat{\sigma}_i^2\}$ is given by twice the inverse of the matrix

$$[\mathrm{tr}(\mathbf{U}_i\mathbf{U}_i'\mathbf{Q}\mathbf{U}_j\mathbf{U}_j'\mathbf{Q})] \qquad \text{where} \quad \mathbf{Q} = \hat{\mathbf{V}}^{-1} - \hat{\mathbf{V}}^{-1}\mathbf{X}(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\mathbf{X}'\hat{\mathbf{V}}^{-1}.$$

Modified maximum likelihood theory with assumed normality gives us the corresponding asymptotic covariance matrix of the $\{\hat{\sigma}_i^2\}$ with $\mathbf{V}$ in place of $\hat{\mathbf{V}}$.

4. Specific Example

This method of analysis was applied to data from an unbalanced grazing trial involving 12 treatments and 105 observations using a total of 19 plots or fields spread over 6 years. The structure of the experiment is shown in Table 1. A detailed description of the experiment can be found in Burns, Harvey, and Giesbrecht (1981) and Burns et al. (1983). One of the characteristics of the experiment is that not all treatments appear in all years, and not all plots are used in all years. In addition, some treatments are shifted to different plots in successive years. Both years and fields are random effects. The fact that individual fields are used for several years means that the error structure is not of the nested type required by Fuller and Battese (1973).

The model used in this analysis is written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{U}_y\mathbf{e}_y + \mathbf{U}_f\mathbf{e}_f + \mathbf{e}$$

where $\mathbf{e}_y$ is the vector of random years effects, $\mathbf{e}_f$ is the vector of random field effects, and $\mathbf{e}$ is the vector of residual errors. The elements of $\mathbf{e}_y$, $\mathbf{e}_f$, and $\mathbf{e}$ are all independent, have mean 0 and variances σ_y^2, σ_f^2, and σ^2, respectively. Although the 105×105 matrix

$$\mathbf{V} = \alpha_y\mathbf{U}_y\mathbf{U}_y' + \alpha_f\mathbf{U}_f\mathbf{U}_f' + \alpha\mathbf{I}$$

with $\alpha_y \geq 0$, $\alpha_f \geq 0$, and $\alpha > 0$ can be inverted numerically, it was more efficient to compute

$$\mathbf{X}'\mathbf{V}^{-1}\mathbf{X} = \mathbf{X}'\mathbf{V}_f^{-1}\mathbf{X} - \alpha_y\mathbf{X}\mathbf{V}_f^{-1}\mathbf{U}_y(\mathbf{I}_6 + \alpha_y\mathbf{U}_y'\mathbf{V}_f^{-1}\mathbf{U}_y)^{-1}\mathbf{U}_y'\mathbf{V}_f^{-1}\mathbf{X}',$$

where $\mathbf{I}_6$ is the 6×6 identity matrix and $\mathbf{V}_f^{-1} = (\alpha\mathbf{I} + \alpha_f\mathbf{U}_f\mathbf{U}_f')^{-1}$ is available directly. Only one 6×6 matrix must be inverted numerically.

MINQUE with $\alpha_y = \alpha_f = \alpha = 1$ was used to obtain preliminary estimates of the variance components, $\tilde{\sigma}_y^2$, $\tilde{\sigma}_f^2$, and $\tilde{\sigma}^2$. These were then used as prior values in a MIVQUE analysis to give the final estimates $\hat{\sigma}_y^2$, $\hat{\sigma}_f^2$, and $\hat{\sigma}^2$. Experience showed that further iterations were unnecessary as they did not lead to any appreciable changes. These estimated components

Table 1
Structure of experiment showing relationship of treatments, fields, and years

Treatment	Year 1	Year 2	Year 3	Year 4	Year 5	Year 6
1	A[a], B, C	A, O, C	A, B, C	A, B, C	A, B, C	A, B, J
2	D, E, F	D, E, F	D, E, F	G, H, I	G, H, I	G, H, I
3	K, L, M					
4	N, O, P	Q, B, J				
5	G, H, I	G, H, I	G, H, I			
6	Q, R, J	N, R, P	Q, R, J	Q, R, J	Q, R, J	
7			S, K, L	S, K, L	L	
8			N, M, P	N, M, P	O, M, P	
9				D, E, F	D, E, F	D, E, F
10					N, K	N, K, R
11						Q, M, C
12						O, P, S

[a] Fields are labeled A, B, . . . , S.

were then used to calculate estimates of the fixed effects using generalized Aitken-type least squares, standard errors of the estimates from ordinary least squares and generalized least squares, and approximate degrees of freedom for contrasts. Notice that the contrast between treatments 1 and 2, for example, differs considerably from the contrast of treatment 2 vs the average of treatments 5 and 9. The first is a within year, across fields contrast while the latter is a within field, across years contrast. The differences between the corresponding standard errors should be reflected in different degrees of freedom. Estimates of the ratios σ_y^2/σ^2 and σ_f^2/σ^2 ranged from .25 to 4.

5. Monte Carlo Study

Section 4 provides a complete analysis of the data, but leaves unanswered a number of questions concerning the adequacy of the tests of significance. In particular, one must question the adequacy of using large-sample asymptotic results for such a small experiment. In view of this, two modest simulations were performed using the specific design at hand. Specifically, two sets of 500 repetitions of the experiment were simulated, one with $\sigma_y^2 = \sigma_f^2 = 3.24$ and $\sigma^2 = 1$, and a second with $\sigma_y^2 = \sigma_f^2 = \sigma^2 = 1$. Pseudo-random normal deviates were obtained from the function NORMAL in SAS (Barr et al., 1979, p. 444). This function uses the sum of 12 independent uniform (0, 1) deviates produced by a 64-number shuffle designed to break up autocorrelations (Lewis, Goodman, and Miller, 1969).

A MINQUE step was used in each case to obtain preliminary estimates of the variance components. These were then used as prior values to compute MIVQUE of σ_y^2, σ_f^2, and σ^2. These estimates were then used to define a variance–covariance matrix and compute the generalized least squares analysis. Selected contrasts among ordinary least squares estimates and generalized least squares estimates via (3.1) were computed. Estimates of the respective standard errors were obtained via the matrices $(\mathbf{X}'\mathbf{X})^+\mathbf{X}'\hat{\mathbf{V}}\mathbf{X}(\mathbf{X}'\mathbf{X})^+$ and $(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^+$. Equations (3.2) and (3.3) were used to obtain approximate degrees of freedom for each of the contrasts. It should be emphasized that although the use of estimates as prior values for the variance components in the MIVQUE stage forfeits the property of unbiasedness of $\hat{\sigma}_y^2$, $\hat{\sigma}_f^2$, and $\hat{\sigma}^2$, the estimates of the fixed effects are unbiased.

The variance components estimation is summarized in Table 2. The close agreement between the true values and the means of the 500 simulations suggests that bias is not a serious problem. The poorest agreement is on σ_y^2 and here one must note that the design involved only 6 years and consequently would not be expected to give good estimates of σ_y^2. Estimates of the variances of the estimated components were obtained by substituting $\hat{\mathbf{V}}$ in place of $\mathbf{V}$. Since in the simulation the true components are known, the asymptotic variances, computed using $\mathbf{V}$, are also given. The agreement between the mean of the 500

Table 2
Variance components estimation

	Component	True value	Mean estimate	Mean computed variance	Observed variance	Asymptotic[a] variance
	σ_y^2	3.24	3.33	6.43	4.33	4.43
First set	σ_f^2	3.24	3.25	1.79	1.51	1.57
	σ^2	1.00	1.00	.029	.028	.029
	σ_y^2	1.00	1.04	.70	.46	.47
Second set	σ_f^2	1.00	.99	.22	.20	.21
	σ^2	1.00	1.00	.030	.029	.029

[a] Values computed using the true variance components.

Table 3
Definitions of contrasts and coefficients of σ_y^2, σ_f^2, and σ^2 in the variances of ordinary and generalized least squares estimates of the contrasts

		Contrast number								
		C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9
Treatment	1	−1	−1	0	0	−2	0	−1	1	0
	2	0	0	1	−1	0	−1	−1	0	−1
	3	0	0	0	0	1	0	0	0	0
	4	0	0	0	0	1	0	0	0	0
	5	0	0	0	2	0	0	0	0	0
	6	0	−1	0	0	0	1	1	−1	0
	7	1	0	0	0	0	0	0	0	0
	8	0	0	1	−1	0	0	1	0	1
	9	0	1	−1	0	0	0	−1	−1	1
	10	0	1	−1	0	0	0	1	1	−1
	11	0	0	0	0	0	0	0	0	0
	12	0	0	0	0	0	0	0	0	0
Coefficient[a] in variance of OLS estimate	σ_y^2	.223	1.132	.982	1.056	1.833	.033	.169	.330	.535
	σ_f^2	.620	1.052	.616	1.117	1.327	.429	2.400	.994	.616
	σ^2	.199	.434	.479	.611	.722	.122	.601	.434	.479
Coefficient[b] in variance of GLS estimate using **V** (Simulation 1)	σ_y^2	.000	.005	.003	.006	.003	.000	.000	.000	.001
	σ_f^2	.073	.295	.014	.270	.116	.249	1.024	.257	.010
	σ^2	.636	1.084	.852	1.238	1.638	.208	1.243	.712	.726
Coefficient[b] in variance of GLS estimate using **V** (Simulation 2)	σ_y^2	.002	.036	.022	.041	.020	.001	.002	.003	.005
	σ_f^2	.227	.446	.076	.395	.371	.272	1.205	.317	.057
	σ^2	.357	.772	.719	.975	1.158	.169	.934	.609	.641

[a] Variance formula is

$$\sigma_y^2\mathbf{C}'(\mathbf{X}'\mathbf{X})^+\mathbf{V}_y(\mathbf{X}'\mathbf{X})^+\mathbf{C} + \sigma_f^2\mathbf{C}'(\mathbf{X}'\mathbf{X})^+\mathbf{V}_f(\mathbf{X}'\mathbf{X})^+\mathbf{C} + \sigma^2\mathbf{C}'(\mathbf{X}'\mathbf{X})^+(\mathbf{X}'\mathbf{X})^+\mathbf{C}.$$

[b] Variance formula is

$$\sigma_y^2\,\mathbf{C}'\mathbf{W}'\mathbf{V}_y\mathbf{W}\mathbf{C} + \sigma_f^2\mathbf{C}'\mathbf{W}'\mathbf{V}_f\mathbf{W}\mathbf{C} + \sigma^2\mathbf{C}'\mathbf{W}'\mathbf{W}\mathbf{C},$$

where

$$\mathbf{W} = \mathbf{V}^{-1}\mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^+.$$

computed estimates and the observed empirical variances is very good, especially for $\hat{\sigma}_f^2$ and $\hat{\sigma}^2$.

The contrasts examined in this study are defined in Table 3. They were selected because of the nature of the treatments in the grazing experiment discussed in detail in Burns et al. (1983). They range from contrast 1 which is largely among years and among fields, to contrast 6 which has common years and different fields, and number 3 which is largely an among years, within fields contrast.

A summary contrasting ordinary least squares and generalized least squares estimates is given in Table 4. Two things that should be noted in Table 4 are close agreement between the computed estimates of variance, the empirical observed variances, and the true variances for both sets of estimators, and the fact that the ordinary least squares estimators have much larger variances than the generalized least squares estimators. The conventional wisdom that one can use ordinary least squares but should at least compute the variances properly appears to hold.

The estimates and the associated estimated variances imply tests of significance for both the generalized least squares and the ordinary least squares analyses. For each of the contrasts, $p = G_{\mathrm{df}}(t)$ was computed, where t is the ratio of the estimated contrast to the

Table 4
Estimation of contrasts among fixed effects

	Ordinary least squares				Generalized least squares			
Contrast number	Mean estimate	Mean computed variance	Empirical variance	True[a] variance	Mean estimate	Mean computed variance	Empirical variance	True[a] variance
Simulation 1								
1	−.073	2.96	2.97	2.93	.038	.85	.86	.87
2	−.171	7.62	7.67	7.51	.026	2.03	2.16	2.06
3	.039	5.75	6.08	5.66	−.036	.89	.87	.91
4	.087	7.76	7.68	7.65	−.095	2.11	2.07	2.13
5	.083	11.14	10.17	10.96	.078	1.97	2.00	2.02
6	.092	1.63	1.57	1.62	.041	1.01	1.02	1.02
7	.132	8.97	9.23	8.92	.099	4.55	4.61	4.56
8	.030	4.76	4.99	4.72	−.016	1.54	1.66	1.55
9	−.081	4.26	4.73	4.21	−.001	.75	.79	.76
Simulation 2								
1	−.018	1.05	1.13	1.04	.031	.56	.63	.59
2	.185	2.66	2.53	2.62	.121	1.21	1.30	1.25
3	−.123	2.12	2.00	2.08	−.038	.80	.79	.82
4	.034	2.82	2.38	2.78	.025	1.37	1.34	1.41
5	.017	3.95	3.98	3.88	.077	1.50	1.60	1.55
6	−.081	.58	.58	.58	−.057	.44	.47	.44
7	−.069	3.16	3.09	3.17	−.034	2.10	2.27	2.14
8	.074	1.77	1.94	1.76	−.002	.91	1.00	.93
9	−.090	1.65	1.63	1.63	−.026	.69	.68	.70

[a] True variances are computed using the true variance components which are known in the simulation.

Table 5
Observed Neyman smooth statistic[a] values for significance levels

Contrast number	Ordinary least squares	Generalized least squares
Simulation 1		
1	2.20	2.40
2	4.44	1.34
3	2.70	3.36
4	7.74	3.24
5	8.64	2.30
6	3.11	2.24
7	1.01	1.33
8	5.20	6.10
9	7.98	1.92
Simulation 2		
1	1.42	3.15
2	14.08	7.03
3	11.46	2.22
4	5.22	5.45
5	2.79	4.59
6	8.59	8.99
7	2.01	1.13
8	8.45	2.39
9	6.05	6.46

[a] The Neyman smooth statistic p_4^2, to be compared with χ_4^2.

Table 6
Number of times two-tail $\alpha = .1$ test rejected in 500 trials

Contrast number	Ordinary least squares: Hypothesized value of contrast .6	0	−.6	Generalized least squares: Hypothesized value of contrast .6	0	−.6
Simulation 1						
1	58	51	51	89	56	93
2	49	43	45	64	47	64
3	51	40	40	86	47	65
4	45	43	45	64	50	55
5	33	29	37	62	53	75
6	59	43	73	72	58	72
7	56	50	53	53	57	59
8	52	47	53	79	53	71
9	62	49	50	94	57	92
Simulation 2						
1	81	52	85	105	57	113
2	42	38	59	73	55	87
3	58	35	49	81	48	80
4	38	40	48	73	48	73
5	51	42	52	69	57	83
6	115	52	80	138	55	110
7	54	45	55	64	50	67
8	72	59	69	90	60	72
9	67	43	55	91	46	91

estimated standard deviation, df is the approximate degrees of freedom obtained via (3.2), and $G_n(\cdot)$ is the t distribution with n degrees of freedom. If the test can be treated as a t test, then the p values should be uniformly distributed on the (0, 1) interval. Table 5 gives the Neyman smooth statistic (Kendall and Stuart, 1967, p. 444) computed for the 500 p values computed for each contrast for the two types of estimators. Since the Neyman smooth statistic is distributed as a χ_4^2 random variable, the simulation gives little reason to question the adequacy of the t test for both ordinary and generalized least squares.

The fact that the generalized least squares estimators have smaller variances than the ordinary least squares estimators implies that generalized least squares should lead to more powerful tests. This can be verified by examining Table 6. The entries in this table are counts of the number of times a two-tailed test with $\alpha = .1$ would reject the null hypothesis that the contrast is equal to .6, 0, and −.6. The entries in the column for testing whether the contrast is 0 are indicators of whether the tests of the usual null hypothesis are really performing at the advertised level, while entries in the remaining two columns are indications of power. The conclusion to be drawn is that tests based on generalized least squares may tend to operate at a level slightly above the level of significance advertised (rejection rate under H_0 greater than α) while tests based on ordinary least squares estimators will tend to have a rejection rate slightly less than α. However, these differences are much smaller than the differences in power. Tests based on generalized least squares estimators tend to be considerably more powerful than tests based on ordinary least squares. A comparison of Tables 4 and 6 shows that in both sets of simulations, the ordinary least squares estimate of contrast 5 has relatively large variance. This results in tests that have too few rejections. Contrasts 2, 3, and 4 also tend to have excessive variances in the ordinary least squares analyses.

The conclusions to be drawn from the simulation are as follows:

(i) The bias in the estimates of the variance components is probably not serious.

(ii) The computed variance estimates of the estimated variance components are certainly adequate for $\hat{\sigma}^2$, quite acceptable for $\hat{\sigma}_f^2$ which is based ultimately on 19 fields, and inadequate for $\hat{\sigma}_y^2$ which is based on 6 years.

(iii) The generalized least squares analysis, based on the estimated variance components, is superior to the ordinary least squares analysis. Although both analyses yield unbiased estimates of the fixed effects, the generalized least squares analysis leads to smaller variances and more powerful tests.

(iv) The approximation for the degrees of freedom for the estimated standard errors for the estimated contrasts appear to be reasonable in the sense that the tests of hypothesis perform as expected. This implies that confidence intervals should be adequate.

Résumé

On développe une analyse en deux étapes pour un modèle mixte dans lequel les composantes de la variance dues aux effets aléatoires sont estimées et utilisées pour calculer les estimations des moindres carrés généralisés des effets fixés. On utilise la théorie des grands échantillons pour établir des propriétés asymptotiques. On discute d'une approximation par un test t pour tester les contrastes sur les effets fixés. Deux simulations modestes basées sur un modèle pour un essai de patûrages (Burns, Harvey, and Giesbrecht, 1981, *Proceedings of* 14*th International Grassland Conference*, J. A. Smith and V. W. Hays (eds), 497–500, Boulder, Colorado: Westview Press; Burns et al., 1983, *Agronomy Journal* **75,** 865–871) sont utilisées pour montrer que les résultats asymptotiques sont raisonnables pour de petits échantillons.

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