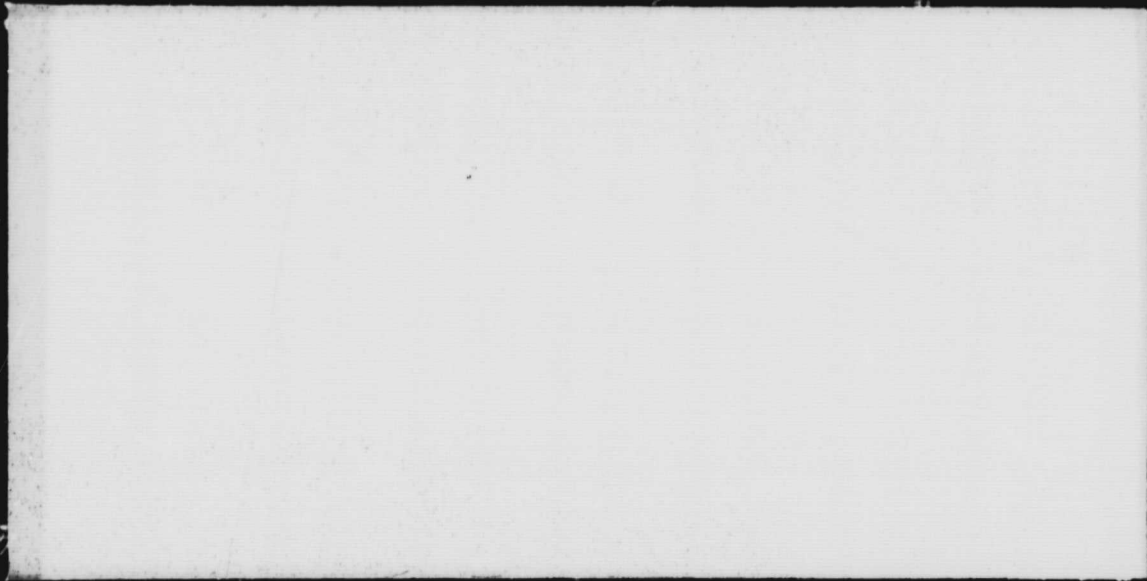


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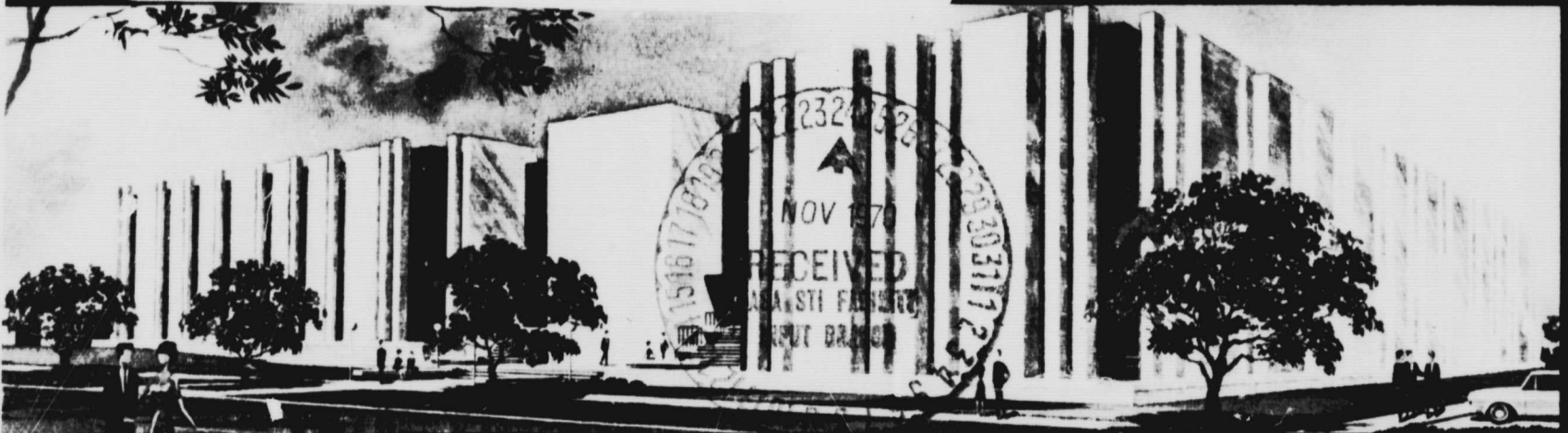
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A COMPUTER PROGRAM FOR THE MIXED ANALYSIS OF VARIANCE
MODEL BASED ON MAXIMUM LIKELIHOOD

by

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CHAPTER I

INTRODUCTION

In this paper we present a computer program for an analysis of variance of unbalanced data assumed to arise from a "mixed model". The analysis is based upon the principle of maximum likelihood estimation developed by Hartley and Rao (1967). In order to fix the ideas it will be necessary to summarize the specification of the model and the estimation theory by maximum likelihood given by these authors. This is done in Sections 1, 2 and 3. Section 4 then spells out in some detail the computational procedure developed. In Section 5, we then proceed to apply the numerical procedure to obtain point estimates of the components of variance involved in the mixed model. The examples chosen comprise both situations for balanced data (when comparison will be made with conventional analysis of variance estimates) as well as unbalanced data. The comparisons for balanced data show excellent agreements for all those situations in which

maximum likelihood estimation agrees with the analysis of variance estimates on theoretical grounds. In the remaining situations good agreement is maintained. Whilst we clearly do not advocate the use of maximum likelihood for balanced data the comparisons should inspire confidence for use with unbalanced data. We should also state here that the doctoral dissertation of one of us (W. K. Vaughn) also contains details of the computer code as well as formulas for the asymptotic variances and covariances of the estimates of the ratios of the components of variance. These are of considerable importance in the estimation of measures of heritability and related studies. It is anticipated that these will be published elsewhere.

CHAPTER II

TECHNIQUES FOR POINT ESTIMATION

2.1 The General Mixed Model

The specification of the general mixed analysis of variance model will be sufficiently general to cover most of the problems arising from unbalanced data. The linear model discussed herein is given by

$$Y = X\alpha + U_1 b_1 + U_2 b_2 + \dots + U_c b_c + e \quad (2.1)$$

where

X is an $n \times k$ matrix of known fixed numbers, $k \leq n$;

U_i is an $n \times m_i$ matrix of known fixed numbers, $m_i \leq n$;

α is a $k \times 1$ vector of unknown constants;

b_i is an $m_i \times 1$ vector of independent variables from $N(0, \sigma_i^2)$;

e is an $n \times 1$ vector of independent variables from $N(0, \sigma^2)$.

The random vectors b_1, b_2, \dots, b_c , and e are mutually independent.

Further it is assumed that the design matrices X and U_i , $i = 1, 2, \dots, c$ are all of full rank. In the model given by (2.1) the fixed effects and random effects are separated so that α contains all levels of all fixed effects and the c random factors are separated so that all elements of b_i have the same variance σ_i^2 .

An additional important assumption about the design matrices is made which assures that the likelihood will tend to zero as any of the ratios $\gamma_1 = \sigma_1^2/\sigma^2$ tends to infinity. See Hartley and Rao [1967]. This is the following assumption of estimability:

Denote by

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

the total number of levels in all c random components. Then the adjoined $n \times (k + m)$ matrix

$$M = [X|U_1|U_2| \dots |U_c]$$

is assumed to have as a base an $n \times r$ matrix W of the form

$$W = [X|U^*]$$

where the $n \times (r - k)$ matrix U^* must contain at least one column from each U_i so that

$$k + c \leq r \leq k + m.$$

2.2 The Likelihood Equations

From the definition of y in (2.1) it is clear that y follows a multivariate normal distribution with mean $X\alpha$ and variance-covariance matrix

$$\sigma^2 H = [I + \gamma_1 U_1 U_1' + \gamma_2 U_2 U_2' + \dots + \gamma_c U_c U_c'] \quad (2.2)$$

where

$$\gamma_i = \sigma_i^2 / \sigma^2. \quad (2.3)$$

Then the likelihood of y is

$$L = (2\pi)^{-\frac{1}{2}n} \sigma^{-n} |H|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2\sigma^2} (y - X\alpha)' H^{-1} (y - X\alpha)\right\}. \quad (2.4)$$

Writing $\lambda = \ln L$

$$\lambda = -\frac{1}{2}n \ln(2\pi) - \frac{n}{2} \ln \sigma^2 - \frac{1}{2} \ln |H| - \frac{1}{2\sigma^2} (y - X\alpha)' H^{-1} (y - X\alpha) \quad (2.5)$$

and differentiating λ with respect to α , σ^2 and γ_i yields the equations

$$\frac{\partial \lambda}{\partial \alpha} = -\frac{1}{2\sigma^2} \{-2 X' H^{-1} y + 2(X' H^{-1} X)\alpha\} = 0 \quad (2.6)$$

$$\frac{\partial \lambda}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} (y - X\alpha)' H^{-1} (y - X\alpha) = 0 \quad (2.7)$$

and

$$\begin{aligned} \frac{\partial \lambda}{\partial \gamma_i} &= -\frac{1}{2} \text{tr}(H^{-1} \frac{\partial H}{\partial \gamma_i}) + \frac{1}{2\sigma^2} (y - X\alpha)' \frac{\partial H^{-1}}{\partial \gamma_i} (y - X\alpha) \\ &= -\frac{1}{2} \text{tr}(H^{-1} U_i U_i') + \frac{1}{2\sigma^2} [(y - X\alpha)' H^{-1} U_i U_i' H^{-1} (y - X\alpha)]. \quad (2.8) \\ &= 0 \end{aligned}$$

The maximum likelihood estimators for α and σ^2 in terms of the unknown γ_i are obtained from equations (2.6) and (2.7). They are

$$\tilde{\alpha}(\gamma_i) = (X'H^{-1}X)^{-1} X'H^{-1}y \quad (2.9)$$

and

$$\tilde{\sigma}^2(\gamma_i) = y'H^{-1}y - y'H^{-1}X(X'H^{-1}X)^{-1}X'H^{-1}y. \quad (2.10)$$

However, the solution of equation (2.8), $\partial \lambda / \partial \gamma_i = 0$ cannot be found explicitly for $\gamma_1, \gamma_2, \dots, \gamma_c$, thus making some numerical technique essential.

2.3 Solution by Steepest Ascent

Substitution of equations (2.9) and (2.10) in (2.8) yields the simultaneous nonlinear equations

$$\begin{aligned} \frac{\partial \lambda}{\partial \gamma_i} \{ \tilde{\alpha}(\gamma_i), \tilde{\sigma}^2(\gamma_i), \gamma_i \} &= -\frac{1}{2} \text{tr} (H^{-1} U_i U_i') \\ &+ \frac{1}{2\tilde{\sigma}^2(\gamma_i)} [y - X\tilde{\alpha}(\gamma_i)] H^{-1} U_i U_i' H^{-1} [y - X\tilde{\alpha}(\gamma_i)] = 0 \end{aligned} \quad (2.11)$$

for the c values of the γ_i .

The solution to this system of equations can be obtained as the asymptotic limits of a system of c simultaneous differential equations, the equations of steepest ascent given by

$$\frac{d\gamma_i}{dt} = \frac{\partial \lambda}{\partial \gamma_i} \{ \tilde{\alpha}(\gamma_i), \tilde{\sigma}^2(\gamma_i), \gamma_i \} \quad (2.12)$$

where the variable of integration, t , is auxiliary and the numerical integration commences at trial values ${}_0\gamma_i$ usually chosen as consistent estimators so the $\gamma_i = {}_0\gamma_i$ at $t = 0$. The solution $\gamma_i(t)$ converges to a solution point $\tilde{\gamma}_i$ which is a root of

$$\frac{d\gamma_i}{dt} = \frac{\partial \lambda}{\partial \gamma_i} = 0 .$$

See Hartley and Rao [1967] for proof of convergence.

A modification of the steepest ascent will ensure that $\gamma_i \geq 0$ along the path of integration. Defining

$$\tau_i = \gamma_i^{1/2} \quad (2.13)$$

which is symmetrical at $\tau_i = 0$, we see that if τ_i is used as a parameter in place of γ_i that

$$\frac{\partial \lambda}{\partial \tau_i} = \frac{\partial \lambda}{\partial \gamma_i} 2\tau_i . \quad (2.14)$$

Thus, the steepest ascent differential equations can be replaced by

$$\frac{d\tau_i}{dt} = \frac{\partial \lambda}{\partial \gamma_i} \{ \tilde{\alpha}(\gamma_i), \tilde{\sigma}^2(\gamma_i), \gamma_i \} 2\tau_i . \quad (2.15)$$

Again, the integration would commence at positive values ${}_0\tau_i$, but should the path of integration reach a point where one or more of the $\tau_i = 0$ the integration would continue along the boundary until the Runge-Kutta procedure would allow the τ_i to again become positive. This procedure ignores and avoids any possible solutions of the likelihood equations with $\tilde{\gamma}_i < 0$.

2.4 Application of the Runge-Kutta Procedure

2.4.1 Polynomial approximation

The technique selected for the numerical integration of the system of c simultaneous differential equations given by equation (2.12) is a fifth order Runge-Kutta procedure. Basically, any Runge-Kutta procedure provides an approximation to a truncated Taylor's series expansion of the independent variables. For the fifth order Runge-Kutta method the approximation is carried out in

such a way that it agrees with the Taylor's series expansion through terms involving h^5 . To apply a fifth order Runge-Kutta procedure to the system of steepest ascent equations it is necessary to evaluate equation (2.11) six times for every iteration. Clearly, since (2.11) involves H^{-1} and since a large number of iterations may be required for convergence, excessive amounts of computer time will be necessary to obtain a solution to the system of equations. For this reason, a second degree polynomial of the form

$$\frac{dr_i}{dt} = b_0^{(i)} + \sum_{j=1}^c b_j^{(i)} \delta_j + \sum_{j=1}^c \sum_{\substack{k=1 \\ j \leq k}}^c b_{jk}^{(i)} \delta_j \delta_k \quad (2.16)$$

is used to approximate the right hand sides of the equations of steepest ascent. Where $b_0^{(i)}$, $b_j^{(i)}$ and $b_{jk}^{(i)}$ are coefficients to be estimated and the δ_j , $j = 1, 2, \dots, c$, represent a coded point on a grid in the delta space. The criterion used to fit the polynomial to the equations of steepest ascent is least squares. The following steps are taken when fitting the polynomial approximation:

(1) Since there are $(c + 1)(c + 2)/2$ coefficients to be estimated at least this many points on the grid in the δ -space must be selected. In fact, one more point on the grid than necessary is used to obtain an estimate of the residuals. The set of points selected must be selected so that the matrix Δ , defined in (3) below has full column rank, that is so $(\Delta' \Delta)^{-1}$ exists.

(2) Defining

0^{τ_i} to be the initial trial value of τ_i for the numerical integration, and

$\Delta_0^{\tau_i}$ to be the grid increment in the τ -space
the points in the τ -space corresponding to the points in the δ -space
are found from the equation

$$\tau_i = \delta_i \Delta_0^{\tau_i} + 0^{\tau_i} \quad (2.17)$$

(3) Defining

F_i to be the right hand side of (2.15) evaluated at the grid points in the τ -space,

Δ to be the matrix of squares and cross products of the delta's whose i^{th} row is

$$[1, \delta_1 \delta_2 \dots \delta_c \delta_1^2 \delta_2^2 \dots \delta_c^2, \delta_1 \delta_2, \delta_1 \delta_3 \dots \delta_{c-1} \delta_c], \text{ and}$$

$\hat{b}^{(i)}$ to be the vector of estimates of the coefficients for the i^{th} equation (2.15), that is

$$\hat{b}^{(i)'} = [\hat{b}_0^{(i)}, \hat{b}_1^{(i)} \hat{b}_2^{(i)} \dots \hat{b}_c^{(i)} \hat{b}_{11}^{(i)} \hat{b}_{22}^{(i)} \dots \hat{b}_{cc}^{(i)} \hat{b}_{12}^{(i)} \hat{b}_{13}^{(i)} \dots \hat{b}_{c-1,c}^{(i)}],$$

the least squares solutions* are found from

*Least squares is used to obtain a mathematical approximation to a mathematical function. The justification of this procedure must be sought by monitoring the truncation error of the approximation obtained.

$$\hat{b}^{(i)} = (\Delta' \Delta)^{-1} \Delta' F_i \quad i = 1, 2, \dots, c \quad (2.18)$$

Upon obtaining the least squares solutions of the coefficients of the polynomial approximation for each equation of the system, a Runge-Kutta procedure is now applied to these approximations. When attaining, via the Runge-Kutta procedure, a set of $\tilde{\tau}_i$ so that

$$|d\tau_i/dt| < \epsilon$$

for every i the procedure terminates. Then, if the estimates of τ_i obtained from the present cycle, say $\tilde{\tau}_i'$, are sufficiently close to the initial trial values for the cycle, say $\tilde{\tau}_i''$, that is if

$$|\tilde{\tau}_i' - \tilde{\tau}_i''| < \epsilon$$

for all values of i , then convergence is established and the estimates of the variances and covariances can be computed. If convergence is not established then the current cycle of the Runge-Kutta procedure is terminated, another polynomial approximation is obtained and with these right hand sides a new Runge-Kutta cycle is started using the terminal values τ_i of the previous cycle as initial trial values for the new cycle.

2.4.2 Selection of optimum step size for Runge-Kutta

The selection of the step size, h , that is the increment in the variable of integration t , in a Runge-Kutta procedure is

important, since it governs the rate of convergence as well as the accuracy of the final solution. For example, if the step size is too small convergence may be very slow. To choose a step size the empirical principle of forcing the second order term in the Taylor's series expansion to be one-tenth the first term was used. This gives for the first order term

$$h \frac{d\tau_i}{dt} = h \frac{\partial \lambda}{\partial \tau_i}$$

and for the second order term

$$\frac{h}{2} \frac{d^2 \tau_i}{dt^2} = \frac{h^2}{2} \left(\frac{\partial^2 \lambda}{\partial \tau_j \partial \tau_i} \right) \frac{\partial \lambda}{\partial \tau_j}$$

Defining

$\left[\frac{\partial^2 \lambda}{\partial \tau_j \partial \tau_i} \right]$ to be the matrix of second partial derivatives of

the log likelihood,

$\left[\frac{\partial \lambda}{\partial \tau_i} \right]$ to be the vector of first partial derivatives of

the log likelihood, and

$\overline{\left[\frac{\partial \lambda}{\partial \tau_i} \right]}$ to indicate the length of $\left[\frac{\partial \lambda}{\partial \tau_i} \right]$ the principle

described above leads to

$$h^2 \left[\frac{\partial^2 \lambda}{\partial \tau_j \partial \tau_i} \right] \left[\frac{\partial \lambda}{\partial \tau_j} \right] = .2h \left[\frac{\partial \lambda}{\partial \tau_i} \right] .$$

Solving for h in terms of lengths of the vectors involved yields

$$h = .2 \left[\frac{\partial \lambda}{\partial \tau_i} \right] / \left[\frac{\partial^2 \lambda}{\partial \tau_j \partial \tau_i} \right] \left[\frac{\partial \lambda}{\partial \tau_j} \right] .$$

More explicitly we obtain for the vectors and matrices involved

$$\left[\frac{\partial \lambda}{\partial \tau_i} \right]_{\delta=0} = [b_0^{(1)}, b_0^{(2)}, b_0^{(3)}, \dots, b_0^{(c)}] ,$$

$$\left[\frac{\partial^2 \lambda}{\partial \tau_j \partial \tau_i} \right]_{\delta=0} = \begin{bmatrix} \frac{b_1^{(1)} 2\tau_1}{\Delta_0 \gamma_1} & \frac{b_2^{(1)} 2\tau_2}{\Delta_0 \gamma_2} & \dots & \frac{b_c^{(1)} 2\tau_c}{\Delta_0 \gamma_c} \\ \frac{b_1^{(2)} 2\tau_1}{\Delta_0 \gamma_1} & \frac{b_2^{(2)} 2\tau_2}{\Delta_0 \gamma_2} & \dots & \frac{b_c^{(2)} 2\tau_c}{\Delta_0 \gamma_c} \\ \vdots & \vdots & \dots & \vdots \\ \frac{b_1^{(c)} 2\tau_1}{\Delta_0 \gamma_1} & \dots & \dots & \frac{b_c^{(c)} 2\tau_c}{\Delta_0 \gamma_c} \end{bmatrix} ,$$

and

$$\left\{ \left[\frac{\partial^2 \lambda}{\partial \tau_i \partial \tau_i} \right] \left[\frac{\partial \lambda}{\partial \tau_i} \right] \right\} = \left[\sum_{i=1}^c \frac{2b_0^{(i)} b_i^{(1)} \tau_i}{\Delta_0 \gamma_i} , \sum_{i=1}^c \frac{2b_0^{(i)} b_i^{(2)} \tau_i}{\Delta_0 \gamma_i} , \dots , \sum_{i=1}^c \frac{2b_0^{(i)} b_i^{(c)} \tau_i}{\Delta_0 \gamma_i} \right] .$$

These expressions lead to the following optimum h for the numerical integration

$$h = \frac{.2 \sqrt{\sum_{i=1}^c (b_0^{(i)})^2}}{\sqrt{\sum_{i=1}^c \left[\sum_{j=1}^c \frac{2b_0^{(j)} b_1^{(i)} \tau_{j1}}{\Delta_0 \tau_j} \right]^2}}$$

A computer program has been implemented making use of the above derivations to solve the likelihood equations (2.6), (2.7), (2.8). Documentation for the computer program is given in Chapter V.

CHAPTER III

EXAMPLES FOR POINT ESTIMATION

3.1 Introduction

This section is concerned with applying the techniques derived in sections 2.1 to 2.4 to specific examples. The majority of the examples are small, balanced data examples to facilitate comparisons between maximum likelihood and analysis of variance estimators. While analysis of variance estimators are unbiased, such is not always the case with maximum likelihood, but agreement between analysis of variance and maximum likelihood is obtained, in the balanced case, when maximum likelihood yields unbiased estimators.

3.2 The Two-Fold Nested Model

Snedecor and Cochran [1967 p. 286] cite data on the calcium concentration in turnip greens. Four plants were taken at random, then three leaves were randomly selected from each plant. From each leaf two samples of 100 mg. each were taken and the calcium content was determined by microchemical methods giving rise to the data in Table 3.1.

Table 3.1

Calcium Concentration in Turnip Greens				
Plant	Leaf	Determinations		
1	1	3.28	3.09	
	2	3.52	3.48	
	3	2.88	2.80	
2	1	2.46	2.44	
	2	1.87	1.92	
	3	2.19	2.19	
3	1	2.77	2.66	
	2	3.74	3.44	
	3	2.55	2.55	
4	1	3.78	3.87	
	2	4.07	4.12	
	3	3.31	3.31	

The model used for this analysis is

$$y_{ijk} = \mu + a_i + b_{ij} + e_{ijk} \quad (3.1)$$

where

a_i represents the effect of the i^{th} level of plants,

b_{ij} represents the effect of j^{th} leaf from the i^{th} plant,

e_{ijk} is the effect of the k^{th} determination from the j^{th} leaf from the i^{th} plant, and $i = 1, 2, 3, 4,$

$j = 1, 2, 3,$ and $k = 1, 2.$

The following assumptions are made:

$$a_i \sim N(0, \sigma_a^2),$$

$$b_{ij} \sim N(0, \sigma_b^2),$$

$$e_{ijk} \sim N(0, \sigma_e^2),$$

a_i , b_{ij} , and e_{ijk} are all mutually independent.

Table 3.2 gives the analysis of variance for the above data.

Table 3.2

Analysis of Variance for Turnip Green Data			
Source of Variation	d.f.	Mean Square	EMS
Plants	3	2.520115267	$\sigma_e^2 + 2\sigma_b^2 + 6\sigma_a^2$
Leaves/Plants	8	.328775	$\sigma_e^2 + 2\sigma_b^2$
Determinations/Leaves	12	.0066541667	σ_e^2

The analysis of variance estimates can be obtained from Table 3.2 by equating the mean square column to the expected mean square column and solving for the unknown parameters. This gives

$$\hat{\sigma}_a^2 = (2.520115267 - .328775)/6 = .3652233778$$

$$\hat{\sigma}_b^2 = (.328775 - .0066541667)/2 = .1610604167, \text{ and}$$

$$\hat{\sigma}_e^2 = .0066541667.$$

From these we obtain the estimates of γ_a and γ_b as $\hat{\gamma}_a = 54.8864$ and $\hat{\gamma}_b = 24.204$.

The two-fold nested model given by (3.1) may be rewritten using the notation of equation (2.1) as

$$y = X\mu + U_1 b_1 + U_2 b_2 + e \quad (3.2)$$

where

$$n = 24, m_1 = 4, m_2 = 12, c = 2, k = 1,$$

and where X is the 24 element unitary column vector and U_1 and U_2 are the usual 24×4 and 24×12 design matrices of 1's and 0's representing 'Plants' and 'Leaves within plants' respectively. Finally the vectors of effect variables b_1 and b_2 are defined by

$$b_1' = [a_1, a_2, a_3, a_4], \text{ and}$$

$$b_2' = [b_{11} b_{12} b_{13} b_{21} b_{22} b_{23} b_{31} b_{32} b_{33} b_{41} b_{42} b_{43}].$$

To obtain the maximum likelihood estimates for the parameters of the mixed model several complete Runge-Kutta cycles, that is refitting of the polynomial approximation, were necessary to achieve convergence for this example. The first complete cycle will be discussed in detail. The steps of this cycle are:

- (1) All necessary constants and design matrices as well as the δ -grid are input to the computer program.

From the δ -grid the τ -grid is obtained using the initial trial values ${}_0\tau_1 = (39)^{\frac{1}{2}}$, ${}_0\tau_2 = (24)^{\frac{1}{2}}$ and the grid increments $\Delta_0\tau_1 = 5$, and $\Delta_0\tau_2 = 5$.

- (2) From ${}_0\tau_1$ and ${}_0\tau_2$ initial values of $\tilde{\alpha}({}_0\tau_1)$ and $\tilde{\sigma}^2({}_0\tau_1)$ are obtained. For this example they are $\tilde{\alpha}({}_0\tau_1) = 3.0121$ and $\tilde{\sigma}^2({}_0\tau_1) = .0066612$.
- (3) Using the estimates of α and σ^2 together with the grid obtained from the initial trial values of the τ_i and the grid increments the polynomial approximations are obtained as described above. For the first cycle for this example they are:

$$\begin{aligned} \frac{d\tau_1}{dt} = & .000157 - .0474\delta_1 + .0217\delta_2 + .00616\delta_1^2 \\ & - .00619\delta_2^2 + .000895\delta_1\delta_2 \end{aligned} \quad (3.3)$$

$$\begin{aligned} \frac{d\tau_2}{dt} = & .00793 + .0168\delta_1 - .214\delta_2 - .000105\delta_1^2 \\ & + .0506\delta_2^2 - .0082\delta_1\delta_2 \end{aligned} \quad (3.4)$$

- (4) The Runge-Kutta procedure is now applied to this system of differential equations yielding, at the end of the first cycle, ${}_1\tilde{\gamma}_1 = 39.093$, ${}_1\tilde{\gamma}_2 = 24.19$, ${}_1\tilde{\sigma}_e^2 = .00666$ and ${}_1\tilde{\mu} = 3.0121$.

- (5) Since convergence has not been established another cycle is started with the initial trial values obtained from (4) above.

For this example a total of three complete cycles were necessary to establish convergence. The number of cycles required for convergence may vary and will always depend on the initial trial values for the first cycle. For this example the final values were $\tilde{\gamma}_a = 39.095$, $\tilde{\gamma}_b = 24.1999$, $\tilde{\sigma}_e^2 = .0066549$ and $\tilde{\mu} = 3.0121$.

It is well known that the analysis of variance procedure produces estimates that are unbiased. While in some cases maximum likelihood also provides unbiased estimates there is no guarantee that this is the case. In this example it is obvious that $\tilde{\gamma}_a$ is biased while $\tilde{\gamma}_b$ as well as $\tilde{\sigma}_e^2$ are unbiased. Hartley and Rao [1967] show that their procedure gives the following maximum likelihood estimates for the balanced two-fold nested model of example one:

$$4(\tilde{\sigma}_e^2 + 2\tilde{\sigma}_b^2 + 6\tilde{\sigma}_a^2) = \sum_{ijk} (\bar{y}_{1..} - \bar{y}_{...})^2, \quad (3.5)$$

$$(\tilde{\sigma}_e^2 + 2\tilde{\sigma}_b^2) = \sum_{ijk} (\bar{y}_{1j.} - \bar{y}_{1..})^2/8, \quad (3.6)$$

$$\tilde{\sigma}_e^2 = \sum_{ijk} (y_{ijk} - \bar{y}_{1j.})^2/12. \quad (3.7)$$

Table 3.3

Comparison of Maximum Likelihood and Analysis of Variance
Estimators for Turnip Green Data

	γ_a	γ_b	σ_e^2
A.O.V.	54.8864	24.204	.0066542
M.L.E. FROM Computer Program	39.095	24.1999	.0066549
M.L.E. FROM Table (3.2)	39.106	24.204	.0066542

We see from Table 3.3 that the analysis of variance estimate of γ_a and the maximum likelihood estimate of γ_a are not the same. As was indicated in equation (3.5) this happens because the maximum likelihood estimate is biased. However, if the sum of squares for plants in line one of Table 3.2 is divided by 4 instead of 3, thus making the analysis of variance estimate comparable to maximum likelihood, we see from lines 2 and 3 of Table 3.3 that there is very close agreement between $\tilde{\gamma}_a$ obtained from the two different methods. Since maximum likelihood gives unbiased estimates of γ_b and σ_e^2 there is no need for this adjustment for comparison. In all cases where the maximum likelihood estimate should agree with the analysis of variance estimate the two agree to at least two decimal places and the estimates of the error mean square agree to five places. Indeed, if a more stringent criterion for convergence is imposed in the computer program better

agreement can be attained. Although this technique of maximum likelihood does not guarantee a global maximum of the likelihood function for this example it was in fact obtained.

3.3 Unbalanced One-Way Classification

Ostle [1963 p. 287] cites data on the moisture content of pine boards. Five storage conditions are studied to determine the effect on the moisture content of white pine lumber. Table 3.4 gives the data arising from this example.

Table 3.4

Moisture Content of Fourteen Pine Boards				
Storage Conditions				
1	2	3	4	5
7.3	5.4	8.1	7.9	7.1
8.3	7.4	6.4	7.5	
7.6	7.1		10.0	
8.4				
8.3				

The model used to analyze this data is

$$y_{ij} = \mu + a_i + e_{ij} \quad (3.8)$$

where

a_i represents the effect of the i^{th} level of storage conditions,

e_{ij} represents the effect of the j^{th} board subjected to the i^{th} storage condition, $i = 1, \dots, 5$, $j = 1, 2, \dots, n_i$,

$$a_i \sim N(0, \sigma_a^2),$$

$$e_{ij} \sim N(0, \sigma_e^2), \text{ and}$$

a_i and e_{ij} are all mutually independent.

The analysis of variance for this data is given in Table 3.5.

Table 3.5

Analysis of Variance for Pine Board Data			
Source of Variation	d.f.	Mean Squares	EMS
Storage Conditions	4	2.67	$\sigma_e^2 + 2.64\sigma_a^2$
Experimental Error	9	.80	σ_e^2

The analysis of variance estimates for σ_a^2 , σ_e^2 and γ_a are $\hat{\sigma}_a^2 = .70$, $\hat{\sigma}_e^2 = .80$ and $\hat{\gamma}_a = .87$.

Writing the model (3.1) using the notation of (2.1) we have

$$y = X\mu + U_1 b_1 + e$$

where $n = 14$, $m_1 = 5$, $c = 1$, $k = 1$, and X is the 14 element

unitary vector and U_1 the 14×5 design matrix representing storage conditions whilst

$$b_1 = [a_1, a_2, a_3, a_4, a_5] .$$

For the initial cycle for this example the trial value chosen was ${}_0\tau_1 = ({}_0\gamma_1)^{1/2} = (.9)^{1/2}$ and the grid increment was $\Delta_0\tau_1 = .85$. Table 3.6 gives a concise presentation of what happens during each cycle for this example.

Table 3.6

Runge-Kutta Cycles for Pine Board Data

Cycle	$\tilde{\gamma}_1$	Polynomial Approximation*
0	.9	$-.4518 - 1.520\delta_1 + .7145\delta_1^2$
1	.675	$-.154 - .622\delta_1 - .444\delta_1^2$
2	.402	$.852 - .971\delta_1 + .115\delta_1^2$
3	.669	$.00804 - .703\delta_1 + .156\delta_1^2$
4	.672	$.000316 - .699\delta_1 + .155\delta_1^2$
5	.673	$.000077 - .699\delta_1 + .155\delta_1^2$

*These approximations change from cycle to cycle because of the changes in origin and width of the grid in the τ -space resulting in different $\tau - \delta$ relations.

Table 3.7 gives a comparison of the analysis of variance and maximum likelihood estimates for this example.

Table 3.7

Comparison for One-Way Classification		
	γ_1	σ_e^2
Analysis of Variance	.87	.70
Maximum Likelihood	.673	.773

Comparisons between maximum likelihood and analysis of variance is difficult for unbalanced data. Even for this simplest case of the one-way classification the likelihood equations cannot be solved explicitly for the estimates of σ_a^2 and σ_e^2 and hence, γ_a . However, for this example maximum likelihood does not give answers too different from those from the customary analysis of variance.

3.4 Two-Fold Nested Model When One Variance Ratio is Zero

Snedecor and Cochran [1967 p. 289] cites data on pig breeding. Five sires are to be evaluated in pig raising. Each sire is mated to a random group of dams, each mating producing a litter of pigs. Table 3.8 gives the average daily gain of two pigs from each litter.

Table 3.8

Average Daily Gain of Two Pigs				
Sire	Dam	Pig Gains		
1	1	2.77	2.38	
	2	2.53	2.94	
2	1	2.28	2.22	
	2	3.01	2.61	
3	1	2.36	2.71	
	2	2.72	2.74	
4	1	2.87	2.46	
	2	2.31	2.24	
5	1	2.74	2.56	
	2	2.50	2.48	

In this example Snedecor regarded 'sires' as a fixed effect. However, for purposes of illustrating the maximum likelihood technique when one variance ratio is zero, the same model and assumptions are used as in section 3.2 equation (3.1). Table 3.9 gives the analysis of variance for this data.

Table 3.9

Analysis of Variance for Pig Data			
Source of Variation	d.f.	Mean Square	EMS
Sires	4	.0249325	$\sigma_e^2 + 2\sigma_b^2 + 4\sigma_a^2$
Dams-Same Sire	5	.11271	$\sigma_e^2 + 2\sigma_b^2$
Pairs-Same Dam	10	.0387	σ_e^2

Analysis of variance estimates of σ_a^2 , σ_b^2 and σ_e^2 are obtained as above. Since the mean square for dams within sires is larger than the mean square for sires the analysis of variance method gives a negative estimate for σ_a^2 . The estimate generally used when this happens is $\hat{\sigma}_a^2 = 0$. We can then obtain the estimates of σ_b^2 in two ways as follows:

- (1) The estimate, $\hat{\sigma}_b^2$, can be obtained from

$$1\hat{\sigma}_b^2 = (.11271 - .0387)/2 = .037005$$

which is the usual analysis of variance estimate.

- (2) Since $\hat{\sigma}_a^2 = 0$, and assuming this implies $\sigma_a^2 = 0$, the mean square for sires has the same expectation as the mean square for dams - same sire. This suggests a pooling of the two sums of squares which gives

$$2\hat{\sigma}_b^2 = (.073698 - .0387)/2 = .017499 .$$

From these two estimates $\hat{\gamma}_b$ and $\hat{\gamma}_b$ are

$$\hat{\gamma}_b = .9562$$

and

$$\hat{\gamma}_b = .45217 .$$

Turning now to the computer program for this example the initial trial values were $\tau_a = (\gamma_a)^{1/2} = (1)^{1/2}$, $\tau_b = (\gamma_b)^{1/2} = 1$, $\Delta \tau_b = 1$ and $\Delta \tau_b = .9$. From these initial trial values four complete cycles were required to establish convergence. The final maximum likelihood estimates are $\tilde{\gamma}_a = 0$, $\tilde{\gamma}_b = .35696$, $\tilde{\sigma}_e^2 = .0387$ and $\tilde{\mu} = 2.5740$. The computer program solves the equations (2.7) and (2.14) and since $\tilde{\gamma}_a = 0$ the computer program solves the equations $\frac{\partial \lambda}{\partial \sigma^2} = 0$, $\frac{\partial \lambda}{\partial \gamma_b} = 0$ and $\tilde{\gamma}_a = 0$. Now Hartley and Rao [1967 p. 100-101] spell out the above likelihood equations for the special case of a balanced two-fold nested model. For $\tilde{\sigma}_b^2$ we have

$$\tilde{\sigma}_b^2 = \frac{1}{pq} \left\{ d_2' d_2 + m q \tilde{\sigma}^2 \frac{\tilde{\gamma}_b}{1+r\tilde{\gamma}_b} \left[1 + \frac{r^2 \tilde{\gamma}_a \tilde{\gamma}_b}{1+r\tilde{\gamma}_b+q r \tilde{\gamma}_a} \right] \right\}$$

where

$$d_2' d_2 = \left(\frac{r \tilde{\gamma}_b}{1+r\tilde{\gamma}_b} \right)^2 \sum_{ij} (\bar{y}_{ij} - \bar{y}_{i..})^2 + \left(\frac{r \tilde{\gamma}_b}{1+r\tilde{\gamma}_b+q r \tilde{\gamma}_a} \right)^2 q \sum_i (\bar{y}_{i..} - \bar{y} \dots)^2 .$$

Since $\gamma_e = 0$ this reduces to

$$\begin{aligned} \tilde{\sigma}_b^2 = \frac{1}{pq} & \left\{ \left(\frac{r\tilde{\gamma}_b}{1+r\tilde{\gamma}_b} \right)^2 \sum_{ij} (\bar{y}_{1j\cdot} - \bar{y}_{1\cdot\cdot})^2 \right. \\ & \left. + \left(\frac{r\tilde{\gamma}_b}{1+r\tilde{\gamma}_b} \right)^2 q \sum_1 (\bar{y}_{1\cdot\cdot} - \bar{y}\dots)^2 + \frac{\tilde{\gamma}_b}{1+r\tilde{\gamma}_b} pq \tilde{\sigma}^2 \right\} \end{aligned}$$

which leads to

$$\tilde{\sigma}_e^2 + r\tilde{\sigma}_b^2 = \frac{1}{mq} \left\{ r \sum_{ij} (\bar{y}_{1j\cdot} - \bar{y}_{1\cdot\cdot})^2 + qr \sum_1 (\bar{y}_{1\cdot\cdot} - \bar{y}\dots)^2 \right\}$$

From these it can be seen that σ_e^2 should be estimated by the 'Pairs/same dam' mean square and $\sigma_e^2 + 2\sigma_b^2$ by the 'pooled mean square' 'Sires + Dams/Same Sire' using the 'wrong' degrees of freedom $5 + 5$ as a divisor. This computation yields exactly $\tilde{\gamma}_b^2 = 0.35695$ confirming the computer program solution exactly. The comparisons are summarized in Table 3.10.

Table 3.10

Comparisons for Pig Data			
	γ_a	γ_b	σ_e^2
AOV ₁	0	.9562	.0387
AOV ₂	0	.45217	.0387
AOV ₃ *	0	.35695	.0387
M.L.E.	0	.35696	.0387

* Based on between dams sum of squares/10.

3.5 Two-Way Classification with Interaction

Bowker and Lieberman [1963 p. 362] cites data on the variability among ovens used in life testing various electronic components. Three ovens and two temperatures normally used for life testing of electronic components are selected. A single type of component is selected and operated in an oven until it fails. Table (3.11) gives the data arising from this experiment

Table 3.11

Electronic Component Data			
	Oven		
	1	2	3
Temperature 550°F	237	208	192
	254	178	186
	246	187	183
600°F	178	146	142
	179	145	125
	183	141	136

The model used for this analysis is

$$y_{ijk} = \mu + a_i + b_j + c_{ij} + e_{ijk}$$

where $i = 1, \dots, A$, $j = 1, 2, \dots, B$, $k = 1, \dots, N$,

$$a_i \sim \text{NID}(0, \sigma_a^2),$$

$$b_j \sim \text{NID}(0, \sigma_b^2),$$

$$c_{ij} \sim \text{NID}(0, \sigma_c^2),$$

$$e_{ijk} \sim \text{NID}(0, \sigma^2),$$

and a_i , b_j , c_{ij} and e_{ijk} are all mutually independent.

Table 3.12 gives the analysis of variance for this data.

Table 3.12

AOV for Electronic Components

Source of Variation	d.f.	Mean Square	EMS
Oven	2	4823.17	$\sigma^2 + 3\sigma_o^2 + 6\sigma_a^2$
Temperature	1	13667.56	$\sigma^2 + 3\sigma_c^2 + 9\sigma_b^2$
Oven \times Temperature	2	137.39	$\sigma^2 + 3\sigma_o^2$
Error	12	69.78	σ^2

From Table 3.12 the analysis of variance estimates are

$$\hat{\gamma}_c = .323$$

$$\hat{\gamma}_b = 21.54$$

$$\hat{\gamma}_a = 11.19$$

$$\hat{\sigma}^2 = 69.78$$

The initial trial values selected for this example are

$$o\tau_a = (o\gamma_a)^{1/2} = (9)^{1/2}, \quad o\tau_b = (o\gamma_b)^{1/2} = (12)^{1/2}, \quad o\tau_c = (o\gamma_c)^{1/2} = (.5)^{1/2}$$

$$\Delta o\tau_a = 5, \quad \Delta o\tau_b = 6, \quad \Delta o\tau_c = .4$$

The polynomial approximations for the first cycle are

$$\begin{aligned} \frac{d\tau_a}{dt} &= .047 - .633\delta_1 + .0879\delta_2 + .026\delta_3 + .391\delta_1^2 \\ &\quad - .04\delta_2^2 - .025\delta_3^2 - .069\delta_1\delta_2 + .0375\delta_1\delta_3 + .036\delta_2\delta_3 , \end{aligned}$$

$$\begin{aligned} \frac{d\tau_b}{dt} &= .0398 + .082\delta_1 - .389\delta_2 + .022\delta_3 - .0349\delta_1^2 \\ &\quad + .23\delta_2^2 - .0189\delta_3^2 - .0557\delta_1\delta_2 + .035\delta_1\delta_3 + .0167\delta_2\delta_3 , \end{aligned}$$

$$\begin{aligned} \frac{d\tau_c}{dt} &= -.31 + .024\delta_1 + .522\delta_2 - .629\delta_3 + .00757\delta_1^2 \\ &\quad - .0267\delta_2^2 + .286\delta_3^2 + .082\delta_1\delta_2 - .082\delta_1\delta_3 - .0187\delta_2\delta_3 . \end{aligned}$$

At the end of the first cycle the revised estimates are

$$\tilde{\gamma}_a = 9.296 , \quad \tilde{\gamma}_b = 12.48 , \quad \tilde{\gamma}_c = .337 .$$

At the end of the fifteenth cycle convergence is established and the maximum likelihood estimates are

$$\tilde{\gamma}_a = 9.54 , \quad \tilde{\gamma}_b = 12.82 , \quad \tilde{\gamma}_c = .326 ,$$

$$\tilde{\sigma}^2 = 69.75 \quad \text{and} \quad \tilde{\mu} = 180.33 .$$

Comparing the maximum likelihood estimates with the analysis of variance estimates we see that $\tilde{\gamma}_c$ and $\hat{\gamma}_c$ and $\tilde{\sigma}^2$ and $\hat{\sigma}^2$ agree

quite well while $\tilde{\gamma}_a$ and $\tilde{\gamma}_b$ do not agree with $\hat{\gamma}_a$ and $\hat{\gamma}_b$. This failure to agree occurs because $\tilde{\gamma}_a$ and $\tilde{\gamma}_b$ are biased.

CHAPTER 1V

DOCUMENTATION FOR THE COMPUTER PROGRAM

4.1 Description of the Program

This chapter is concerned with a description of the computer program mentioned in section 3.2.5. This computer program is designed to obtain the maximum likelihood estimates for the parameters of the mixed analysis of variance model. The computer program, which contains several subroutines, is written in Fortran IV in double precision for the operating system of the I.B.M. 360/65.

The general flow of the program, which is illustrated in figure 4.1 can be described as follows. The main program reads all data necessary to complete the problem including the dimension of the variance-covariance matrix of the observations, the number of variance ratios, the column dimension of the U matrices, the number of points in the grid for the polynomial approximation, the initial estimates of the variance ratios, all design matrices and the observation vector y .

The grid in the gamma space is determined and control is transferred to the subroutine FOFX where the right hand side of (2.15) is evaluated for all grid points. Control is transferred back to the main program where the least squares equations are obtained and then subsequently solved in subroutine SKINNY. Control is then transferred back to the main program where the optimum step

size for the Runge-Kutta procedure is determined. Subroutine RUNGE is entered and the solution to the polynomial approximation (2.16) is determined. Control is transferred back to the main program and if convergence has been established the large sample variance-covariance matrix, is computed. Otherwise a new cycle is started using as initial values the solutions from the previous cycle.

The following is a description of the subroutines used in the computer program.

4.1.1 RUNGE

Subroutine RUNGE is a subroutine designed to solve systems of first order differential equations. The following is a definition of the input parameters to RUNGE.

- (1) N is the number of equations in the system to be solved.
- (2) NN is the number of K values needed for the Runge-Kutta formula. In this case since we are only concerned with a fifth order Runge-Kutta procedure NN is always 6.
- (3) H is the step size for the procedure.
- (4) $XMIN$ is the lower limit for the independent variable.
- (5) $XMAX$ is the upper limit for the independent variable always chosen large.
- (6) $KOUT$ is a variable indicating how frequent along the path of integration the current values of the variance ratios are outputted. For example, if $KOUT$ has the value 5, then on every fifth

iteration the current value of all variance ratios is printed out.

(7) Y is the observation vector.

(8) EPIL is tolerance used to determine if a solution to the system has been found.

(9) XPX is a matrix containing the estimates of b's for the polynomial approximation.

(10) NDEL is the number of b's.

(11) DELGAM is the grid increment in the gamma space.

(12) LERR is an error flag indicating that the path of integration has reached a boundary point. If LERR has the value 1 an error has occurred and an error message so indicates. Otherwise, LERR has the value of zero.

4.1.2 ALFSIG

ALFSIG is the subroutine which computes the value of $\tilde{\alpha}$ and $\tilde{\sigma}^2$ for a given set of $(\gamma_1, \gamma_2, \dots, \gamma_c)$. The input parameters may be described as follows.

(1) X is the full rank design matrix for the fixed effects.

(2) N is the dimension of the variance covariance matrix of the observations.

(3) NX is the number of columns of X.

(4) HINV is the inverse of the variance covariance matrix of observations.

(5) Y is the observation vector.

(6) ALPHAH is the vector of estimates of all fixed effects in the model.

(7) SIGMA2 is the estimate of the error variance.

(8) IRT is an indicator variable so that if IRT = 1 the large sample variance covariance matrix of the fixed effects will be outputted.

4.1.3 FORMH

FORMH is a subroutine which computes H^{-1} as given in (2.2).

This subroutine uses the fact that if Z is the matrix of U_i $i = 1, 2, \dots, c$ adjoined as

$$Z = [\sqrt{\gamma_1} U_1 | \sqrt{\gamma_2} U_2 | \dots | \sqrt{\gamma_c} U_c] \quad (5.1)$$

then

$$H = [I + ZZ']$$

and

$$H^{-1} = I - Z(I + Z'Z)^{-1} Z'$$

necessitating the inversion of only a $\Sigma_{m_i} \times \Sigma_{m_i}$ as opposed to an $n \times n$. A description of the input variables is as follows.

- (1) GAM is the vector of estimates of the variance ratios.
- (2) M is the vector of m_i 's.
- (3) N is the dimension of H.
- (4) U is the three dimensional array of the design matrices

for the random components in the model. The first subscript indicates one of the design matrices U_i $i = 1, \dots, c$ the second and third give the dimensions of that design matrix.

(5) NC is the number of variance components.

(6) HINV is as previously defined.

4.1.4 FOFX

Subroutine FOFX is designed to compute the right hand side of (2.11). The input variables to this subroutine are the same as previously defined with the exception of F. F is the $c \times 1$ vector or right hand sides of (2.15).

4.1.5 FORMZ

Subroutine FORMZ is the subroutine which adjoins the U_i as in equation (4.1) to obtain Z. The input variables are the same as previously defined. Z is the matrix returned to the calling routine.

4.1.6 GTPRD

This subroutine accepts an input matrix A of dimension $NRA \times NCA$ and returns in C a matrix of dimension $NCA \times NCA$ containing $A'A$.

4.1.7 GMPRD

This subroutine receives matrices A of dimension $NRA \times NCA$ and B of dimension $NCA \times NCB$ and returns in C a matrix of dimension $NRA \times NCB$ containing AB.

4.1.8 GMTRA

This subroutine receives a matrix A of dimension $NRA \times NCA$ and returns in B a matrix of dimension $NCA \times NRA$ containing A' .

4.1.9 SKINNY

SKINNY is a subroutine designed to (1) invert real symmetric matrices and (2) to solve systems of simultaneous linear equations with multiple right hand sides. The following is a description of the input parameters to SKINNY.

(1) S is the matrix containing the coefficient matrix in the first N columns.

(2) If a system of equations with K right hand sides is to be solved, the right hand sides are placed in columns $N + 1$ to $N + K = M$ of S.

4.1.10 FOFXR

Using a fifth order Runge-Kutta it is necessary to evaluate the right side of (2.15) six times for every Runge-Kutta iteration. The purpose of FOFXR is to receive the $NDEL \times NC$ matrix of

coefficients and return in $F \frac{d\tau_1}{dt}$.

Presently the program is designed to accept a maximum of 60 observations with 5 variance ratios and no more than 20 levels within each random classification. The maximum length of the alpha vector is 10.

The amount of time needed to solve a problem is difficult to estimate. Certainly, the larger the number of observations the more time will be needed. However, time is also a function of the initial trial values of the variance ratios as well as the step size for the numerical integration.

4.2 Description of Input Data

The following is a description of the control and data cards which are input to the computer program.

(1) Control Card 1 has the format (20I4). Table 4.1 gives the description of card one.

Table 4.1

Control Card I

Column	Variable Name	Item
1-4	N	N is the total number of observations.
5-8	NC	NC is the total number of variance ratios, γ_i .
9-12	NX	NX is the number of columns of the design matrix for the fixed effects.
13-16	NPT	NPT is the number of points on the grid containing the maximum likelihood estimates.

(2) The second card in the data set has format (20A4) and is a header card. Any information the user wishes to print on the first page of output should be punched in this card.

(3) The third card contains the values of m_i for $i = 1, 2, \dots, NC$. This data is punched on this card using format (20I4). Table 4.2 gives the description for this card.

Table 4.2

Control Card III		
Column	Variable Name	Item
1-10	M(1)	M(1) is the number of columns of U_1 .
11-20	M(2)	M(2) is the number of columns of U_2 .
	⋮	
10(c - 1) + 1 - 10c	M(c)	M(c) is the number of columns of U_c .

(4) The fourth card contains the initial trial values of the gammas as well as the grid increments in the gamma space. The format for this card is (8 F 10.5) with $\gamma_1, \dots, \gamma_c$ punched in the first 10c columns and the grid increments punched in the last 10 c columns.

The rest of the data follows in this order.

(5) The design matrices for the random effects are input in numerical order using format (40I2).

(6) The design matrix for the fixed effects is input as X transpose using format (40F2.0).

(7) The $NPT \times NDEL$ matrix Δ as defined in 2.4.1 is input last using format (26F3.0).

Since the program returns to the first read statement at the end of a problem, to indicate the end of all problems the last card should contain 9999 in columns 1-4.

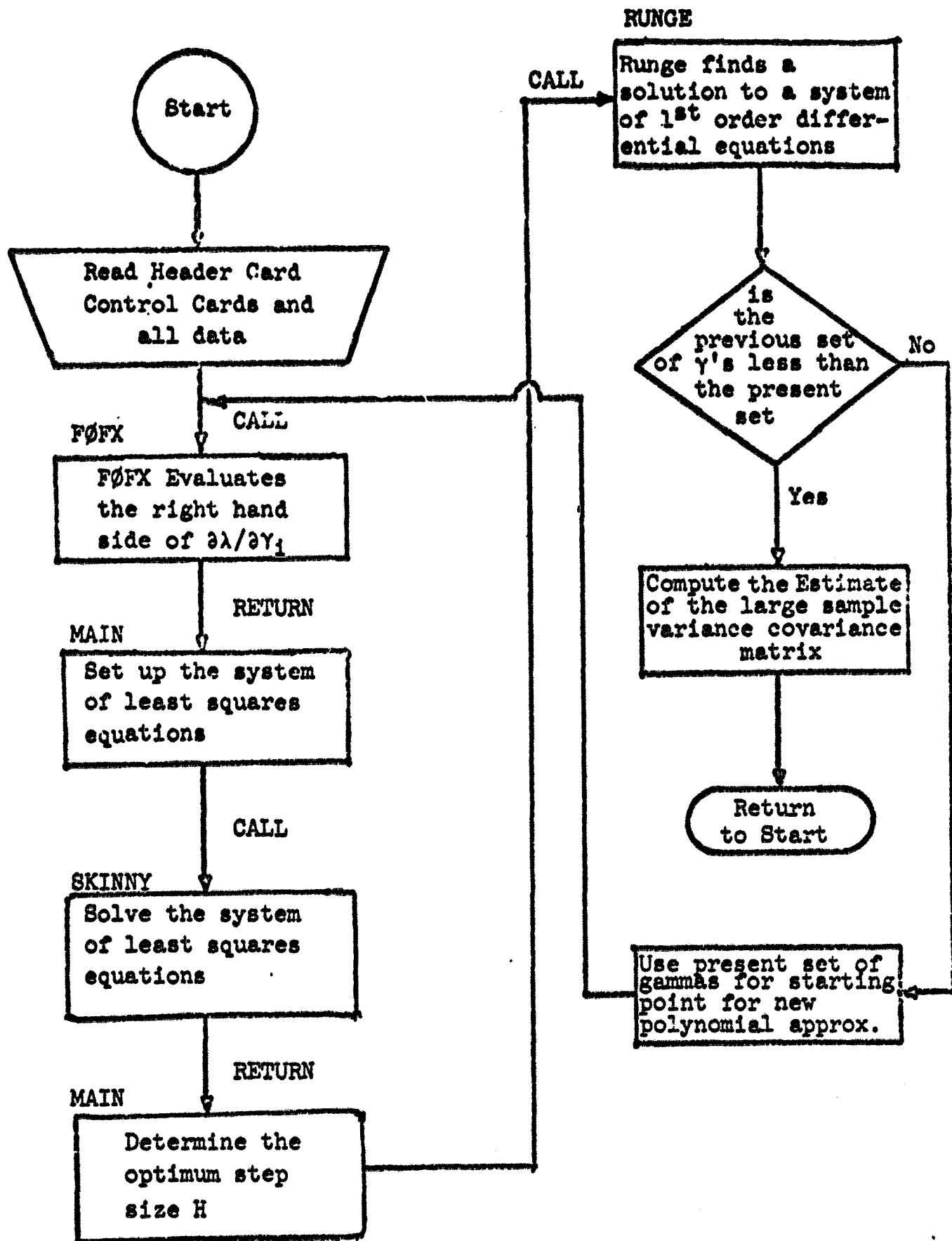


Figure 4.1 Flow of the Program

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