BQUE, AOV and MINQUE procedure in Estimating Variance Components

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Abstracts

Variance components model appears often in designing experiments including time series data analysis. This paper is investigating the properties of the various procedures in estimating variance components for the two-way random model without interaction under normality. In this age of computer-oriented computations, MINQUE is found to be quite practical because of the robustness with respect to the design configurations and parameters. Also adjusted AOV type estimation procedure is found to yield superior results over the unadjusted one.

1. Introduction

The two-way random model without interaction can be repressented as

$$\underline{y} = 1\mu + X_1\underline{\alpha} + X_2\underline{\beta} + \underline{\epsilon} \tag{1}$$

where $\underline{Y}$ is an n-vector of observations, μ is overall mean, X_1 and X_2 are known $n \times a$ $n \times b$ design matrices. The random effects $\underline{\alpha}$ and $\underline{\beta}$ are assumed to have zero mean and variances σ_1^2 and σ_2^2 respectively. The residual error term $\underline{\epsilon}$ is an n-vector with zero mean and variance σ_3^2. All the random effects ($\underline{\alpha}$, $\underline{\beta}$ and $\underline{\epsilon}$) are assumed to be independent of each other. Hence the dispersion matrix of $\underline{Y}$ is given as

$$V^* = \sigma_1^2 X_1 X_1' + \sigma_2^2 X_2 X_2' + \sigma_3^2 X_3 X_3'$$

MINQUE(Minimum Norm Quadratic Unbiased Estmator), proposed by Rao 1972), gives the way simultaneous estimation of σ_1^2, σ_2^2 and σ_3^2 from soloing

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the following sets of linear equations with respect to $\underline{\hat{\sigma}}'=(\hat{\sigma}_1^2, \hat{\sigma}_2^2, \hat{\sigma}_3^2)$,

$$S^*\underline{\hat{\sigma}}=\underline{u},$$

where

$$S^*_{(3\times3)}=\{t(W^*X_iX_i'W^*X_iX_i')\}$$
$$\underline{u}_{(3\times1)}=\{\underline{y}'W^*X_iX_i'W^*\underline{y}\},\ i,j=1,2,3$$
$$w^*=V^{*-1}-V^{*-1}\times(X'V^{*-1}X)^{-1}X'V^{*-1},$$

$x=(X_1;X_2)$, and tr stands for the trace of a rectangualar matrix. Here, V^* involves unknown parameter values (σ_1^2,σ_2^2, and σ_3^2), and Rao himself suggested using the a-priori informations to these parameters.

If we multiply a complete set of orthogonel contrast matrix C of dimension $(n-1)\times n$ to bothsides of (1), we obtain

$$\underline{Z}=C\underline{Y}=CX_1\underline{\alpha}+CX_2\underline{\beta}+C\underline{\epsilon} \qquad (2)$$

It can be shown that both model will yield the same MINQUE. One approach to show this is by proving that in estimating any linear combination of the components, the MINQUE from equation (1) and (2) yield the same matrix, i.e. the matrix A in $\underline{Y}'A\underline{Y}$ from (1) and $C'A^*C$ in $\underline{Z}'A^*\underline{Z}=\underline{Y}'C'A^*C\underline{Y}$ from (2) are identical.

Using this transformed model, the MINQUE of variance components for the two-way random model are obtained from solving the following sets of linear equations for $\underline{\delta}=(\delta_1,\delta_2,\delta_3)$

$$s\ \underline{\delta}=\underline{u} \qquad (3)$$

Where $S=\{tr(W^{-1}V_iW^{-1}V_j)\}$

$\underline{U}=\{\underline{Z}'W^{-1}V_iW^{-1}\underline{Z}\}$

And $W^{-1}=[\text{Variance of } \underline{Z}]^{-1}=[\sigma_3^2(V_3+V_1\sigma_1^2/\sigma_3^2+V_2\sigma_2^2/\sigma_3^2)]$

where $V_i=CX_iX_i'C'$ for $i=1,2,3$.

Noting that (3) is invariant under the sclar multiplication of W, we can reduce the number of unknown parameters from 3 $(\sigma_1^2,\sigma_2^2,\sigma_3^2)$ to 2 $(\sigma_1^2/\sigma_3^2, \sigma_2^2/\sigma_3^2)$.

Denoting the a-priori values of these 2 unknown parameters as r_1^2 and r_2^2, we have the estimating equation for the MINQUE of the two-way random model without interaction as in the following lemma.

Lemma1: The MINQUE, $\underline{\sigma}$, of the variance components for the two-way random model without interaction is obtained by solving the system of linear equations,

$$s\,\underline{\sigma}=u$$

$$s_{(3\times 3)}=\{tr(RV_iRV_i)\}$$

$$\underline{u}'=\{\underline{Z}'RV_iR\underline{Z}\}$$

$$R=[\text{Variance of } \underline{Z}]^{-1}=\sigma_3^{-2}[V_3+r_1^2V_1+r_2^2V_2]^{-1}$$

$$=\sigma_3^{-2}[I_{n-1}-X_eR_m^{-1}X_e']$$

where $$R_m=(\Delta_r^{-1}+X_e'X_e)_{(m\times m)} \text{ and } \Delta_r=\begin{bmatrix} r_1^2I_a & \phi \\ \phi & r_2^2I_b \end{bmatrix}_{(a+b)\times(a+b)}$$

Two types AOV estimators are:

i) row effect adjusted for column effect

ii) both effects not adjusted.

Low(1976) has investigated the properties of the AOV type estimators of the variance components for the two-way random model without interaction. These estimators are obtained from solving the following systems of linear equations with respect to $\underline{\sigma}^A$ (adjusted AOV) and $\underline{\sigma}^u$ (unadjusted AOV).

$$F_A\underline{\sigma}^A=\underline{t}_A,$$

$$F_u\underline{\sigma}^u=\underline{t}_u,$$

where $\underline{t}$'s are (3×1) vector of sum of squares terms in AOV table and 3×3 matrices F's are from their correponding expected values.

2. Variances of the Estimators

Under normality, the MINQUE with correct a-priori values becomes the best quadratic unbiased estimator (BQUE). Since the MINQE and AOV type estimators are all quadratic unbiased, it is reasonable to compare these estimators against the BQUE. To do this, the vairances of the estimator are obtained. Notations used here in are;

n_{ij}; number of observations for (i,j)th cell of the design configuration.

$n_{i.}=\sum_j n_{ij},\ n_j=\sum_i n_{ij}$

$X_c=CX$ where C and X are defined in section 1.

Lemma 2 (Low. 1964): The variances of the AOV adjusted estimators, $\underline{\sigma}^{A\prime}=(\underline{\sigma}_1{}^A,\underline{\sigma}_2{}^A,\underline{\sigma}_3{}^A)$ of the variance components for the two-way random model without interaction are:

$$\mathrm{Var}(\underline{\sigma}_1{}^A)=2\sigma_3{}^4[(n-b)(a-1)/f+2\rho_1{}^2(n-k_4)+\rho_1{}^4k_6]/(n-k_4)^2$$

$$\mathrm{Var}(\underline{\sigma}_2{}^A)=2\sigma_3{}^4[(n-a)(b-1)/j+2\rho_2{}^2(n-k_3)+\rho_2{}^4k_5]/(n-k_3)^2$$

$$\mathrm{Var}(\underline{\sigma}_3{}^A)=2\sigma_3{}^4/f$$

Where

$$j=n-m+1$$

$$k_1=\sum_i n_i{}^2/n \qquad k_2=\sum_j n_j{}^2/n$$

$$k_3=\sum_{ij} n_{ij}{}^2/n_i \qquad k_4=\sum_{ij} n_{ij}{}^2/n_j$$

$$k_5=nk_2-2\sum_{ij} n_{ij}n_{ij}{}^2/n_i+\sum_{jk}(\sum_i n_{ij}n_{ik}/n_i)^2$$

$$k_6=nk_1-2\sum_{ij.} n_{ij}{}^2/n_j+\sum_{ik}(\sum_j n_{ij}n_{ik}/n_j)^2$$

For AOV unadjusted estimators, Searle (1958, 1971 b) gives explicit forms for the variances. However, this invclues a considerable amount of summations and is difficult to visualize. Alternative expressions of the variance forms are given in the following lemma.

Lemma 3: The variances of AOV unadjusted estimators of variance components for the two-way random model without interaction are as follows.

$$\mathrm{Var}(\sigma_2{}^4)=2(f^{23}\sigma_3{}^2)^2\{(n-m)+(n\bar{f}^i)^2(k^2-2k-1)$$
$$-2\bar{f}^i\underline{n}'\Delta_\rho X'X\Delta_i\Delta_\rho\underline{n}+tr[\Delta_i(I_m+\Delta_\rho X'X)]^2\},\ i=1,2,3$$

where

$$k=(\rho_1{}^2\sum_i n_i{}^2+\rho_2{}^2\sum_j{}^2)/n$$

$$\bar{f}^i=(f^{i1}+f^{i2}+f^{i3})/(nf^{i3})$$

$$\Delta_i=(f^{i1}+f^{i3})/f^i\Delta_a+(f^{i2}+f^{i3})/f^{i3}\Delta^q$$

Δ_a and Δ_b are $(a+b)\times(a+b)$ null matrix except the upper a(lower for Δ_b) diagonal elements with 1. Finally the f^{ij}, $i,j=1,2,3$ is the (i,j)th element of the inverse of F^u matrix mentioned in the last part of seetion 1 and this is given as

$$F^u=\begin{bmatrix} n-k_1, & k_3-k_2, & a-1 \\ k_4-k_1, & n-k_2, & b-1 \\ n-k_1, & n-k_2, & n-1 \end{bmatrix}$$

and k_1 k_2, k_3 and k_4 are as given in the lemma 2.

Using the notations Δ and ∇, the variances of MINQUE is given in the following lemma. The detailed derivation is given in Huh (1978).

Lemma 4: Variance of the MINQUE for the two-way random model without interaction is

$$\mathrm{Var}(\sigma_i)=2(\sigma_3{}^2s^{i3})^2\{(n-m-1)+tr(M_i)^2\},\ i=1,2,3$$

where

$$M_i=(I_m+X_e'X_eL_i)(I_m+X^{\circ\prime}X_eL_\rho)$$

$$L_i=R_m{}^{-1}[(s^{i1}/(r_1{}^2s^{i3})-1)\Delta_a+(s^{i2}/(r_2{}^2s^{i3})-1)\Delta_b],$$

$$L_\rho=R_m{}^{-1}[(\rho_1{}^2/r_1{}^2-1)\Delta_a+(\rho_2{}^2/r_1{}^2-1)\Delta_b]$$

$X_e'X_e=X'C'CX$, and s^{ij} is the (i,j)th element of the inverse of (3×3) matrix S given in (3).

It can be noted that $\rho_i{}^2$ appears only through the ratio of $\rho_i{}^2/r_1{}^2$, and for convenience, denote $\xi_i{}^2=r_i{}^2/\rho_i{}^2$.

When a correct set of a=priori values are assigned, i.e.

$\xi_1{}^2=\xi_2{}^2=1$, the MINQUE becomes BQUE and the dispersion matrix is given in the following lemma.

Lemma 5: The dispersion matrix of the BQUE for the two-way random model without interaction is,

$$\mathrm{Var}(\underline{\sigma})=2\sigma_3{}^4S^{-1}$$

where S^{-1} is the inverse of S given in (3).

3. Empirical Investigation

Since the MINQUE procedure of estimation depends on the choice of the a-priori values, the natural question is how robust the estimatior is with respect to the a-priori values. Analytical investigation seems impossible at this stage. Hence empirical results for the representative designs and various combinations of the parameters and their appriori values are given here. The criterion used here is the variance of the estimator relative to the BQUE.

Definition1. (Robustness of the MINQUE)

Robustness of the MINQUE with a-priori values r_1^2 and r_2^2 corresponding to the parameter values ρ_1^2, ρ_2^2 respectively is defined as

$$\upsilon(r^2{}_1,r_2^2\,|\,\rho_1^2,\rho_2^2)=\frac{\text{Variance(MINQUE with } r_1^2,r_2^2)}{\text{Variance(BQUE}\,|\,\rho_1^2,\rho_2^2)}$$

Hence as $\upsilon(r_1^2,r_2^2\,|\,\rho_1^2,\rho^2)$ approaches to 1, the MINQUE is close to the BQUE, and vice versa. Also $\upsilon(r_1^2,r_2^2\,|\,\rho_1^2,\rho_2^2)$ is always greater than or equal to 1. This robustness measure can also be used to investigate the inflation of the variance of AOV type estimators relative to the BQUE.

The following two factors will be considered for the empirical studies.

i) Design configurations: this involves the sample size(n), the number of levels for each factors(a,b) and the $(m\times m)$ matrix $X'X$.

ii) Parameter values (ρ_1^2,ρ_2^2) and their a-priori values (r_1^2,r_2^2).

However from the remark of lemma 4, $\xi_i^2=r_i^2/\rho_i^2$, $i=1,2$ will be used instead of r_1^2 and r_2^2. This is advantageous from the comsideration that the choices of the various combinations of the four parameters $(r_1^2,r_2^2,\ \rho_1^2,\rho_2^2)$ can be reduced by the appropriate salection of the new parameters, ξ_1^2, ξ_2^2, ρ_1^2 and ρ_2^2.

To implement the disign matrix $X'X$ into the empirical studies, a measure of unbalancedness is introduced. Here the Eucledian norm of $X'X$ will the used, and define the measure of unbalancedness as in the following.

Definition2.

Define

$$u(X)=[(tr(X'X)^2-\underset{x}{\text{Min}}\ tr(X'X)^2)/(\underset{x}{\text{max}}\ tr(X'X)^2-\underset{x}{\text{min}}\ tr(X'X)^2)]$$

as a measure of unbalancedness for a given set of sample size (n) and number of levels for the main factors (a,b). The minimum and maximum with respect to X means that the design matrix is as much balanced (unbalanced) as possible for a given set of parameters (n,a,b). Also tr means the trace of the matrix.

The rationale and more deseriptions on this measure are given in Huh (1978).

Emprical studies has shown the following.

i) $0.0<\mu(x)<0.1$, almost balanced

ii) $0.1<\mu(x)<0.3$, unbalanced

iii) $0.3<\mu(x)<1.0$, extremely unbalanced.

The design configuration with $\mu(x)=1$ is as following.

1 1 ⋮ 1	ϕ
$n-a-b+2$	1 1 …… 1

and this matrix is referred to as L-type design(1963). Since the variances of the AOV type estimators considered in lemma 2 and 3 work only for the connected designs, the choice of the designs are constrained to the case of the connected designs.

4. Choice of Design Configurations

Choice of the design configurations are hence based upon the factors n,a,b and $\mu(x)$ as;

n : (15, 30, 150)

a,b : (3, 5, 7)

$\mu(x)$: (almost balanced, unblanced, extremely unblanced).

The 1/9 fractional factorial experiment is introduced and the following 9 designs are selected for the empirical studies, where the numbers in the rectangle reprensents the number of observations and blank is the empty cells.

D1 (3, 3, 15, 0.0)

2	1	2
2	2	1
1	2	2

D2 (5, 7, 15, 0.17)

1	1	1					
	1	1	1				
		1	1	1			
			1	1	1		
				1	1	1	
					1	1	1

D3 (7, 5, 15, 0.56)

1				
1				
1	1			
1	1			
1	1			
1	1			
1	1	1	1	1

D4 (5, 5, 30, 0.0)

1	1	1	1	2
1	1	1	2	1
1	1	2	1	1
1	2	1	1	1
2	1	1	1	1

D5 (7, 5, 30, 0.22)

2		
2	2	
2	2	2
2	2	3
	2	3
		3
		3

D6 (3, 7, 30, 0.38)

1	1	1				
2	2	2				
3	3	3	3	3	3	3

D7 (7, 7, 150, 0.0)

3	3	3	3	3	3	3
3	3	3	3	3	3	3
3	3	3	3	3	3	3
3	3	3	3	3	3	3
3	3	3	3	3	3	4
3	3	3	3	3	4	3
3	3	3	3	4	3	3

D8 (3, 5, 150, 0.20)

10	10	10		10
	10	10	20	
20		10	20	20

D9 (5, 3, 150, 0.36)

10		
10		
10	10	
10	10	
30	30	30

The numbers in the parenthesis represent the values of $(a, b, n, \mu(x))$.

For the parameter values, 3 different values for ρ_i^2 (0.1, 1.0, 10.0) and

5 different values for ξ_i^2(0. 1, 0. 5, 1. 0, 2. 0, 10. 0) For $i=1, 2$ were chosen. This choice will make 225 ($3\times3\times5\times5$) different combinations for each 9 designs.

4. Empirical Results

In general, empirical studies has shown that when the main effect component being estimated is smaller than the error component, the resulting estimator gave larger sampling variance relative to the case when the main effect component is large than the error component.

The AOV adjusted method yielded sampling variances close to those of the BQUE while the AOV unadjusted method gave very poor estimators for most of the cases considered.

The MINQUE method was found to he very robust for all practical purposes. The robustness was especially dominant when the main effect component is relatively larger to the error component. This is often the case in practice.

For the convenience of the investigation of the result, the variances of the estimators were divided by the square of the corresponding components, i.e., $\mathrm{Var}(\hat{\sigma}_i^2)/\sigma_i^4$ for $i=1, 2, 3$. The vertical scale of the efficiency plots are base 10 log-scaled and the values are the actual ones.

4. 1. Properties of the BQUE.

a) Estimating the main component. (refer to PLOT 1)

When the main effect being estimated is small relative to the error variance component (i.e, when $\xi_i^2=0.1$), the BQUE showed large variances compared to the reverse case. This phenomenon becomes more evident when the sample size gets smaller. The effect of the change of design configuration for the given sample size was a rather interesting one. As the design approaches more balanced, the change in the efficiencies remained more stable relative to the change in the effciencies of the designes with high values of $\mu(x)$ (x), i.e. more unbalanced design configurations.

b) Estimating the error component (refer to PLOT 2)

As is evident from the PLOT 2, the variance of the error component estimator did not depend much on the magnitude of the main effect components. As in the case of the main effect component estimation, the variance of the estimator gets inflated as the sample size gets smaller. For the given set of sample sizes, the estimator yielded larger variance as the sum of the levels of row and column gets larger. This is intuitively appealing since the degree of freedom for the error term gets smaller when the levels of the main effects gets larger.

4.2. Properties of the AOV estimutor. (Refer to the Appendix)

For most of the cases investigated, the AOV adjusted estimator yielded better results than the AOV unadjusted estimator both for the main effect and error component. Some specific points are:

i) For the layputs with obsevations clustered in the neighbor of diagonal (D2, D5), it is not clear which estimator is preferable for the main effect component estimation.

ii) In estimating σ_1^2 when $\sigma_1^2/\sigma_3^2=10$ for the layouts of L-type and staggered type (D3, D6, D9), the AOV estimators were at least 5% off from the BQUE. Especially for D9, the AOV adjusted was over 30% from the BQUE.

iii) When estimating σ_1^2, the AOV adjusted estimator yielded smaller variance as the σ_2^2 gets larger. The AOV unadjusted estimator yielded the opposite results.

iv) For the estimation of error component, AOV adjusted estimator is strongly recommended. The remark iii) applies also to the estimation of error component.

v) Except for the layouts of D2 and D3, the AOV adjusted estimator of error yielded variances almost close to that of the BQUE. The BQUE of the error component of D2 and D3 were noted to be the worst cases out of the 9 layouts considered.

4. 3. Robustness of the MINQUE (Refer to the Appendix)

The MINQUE is quite robust for the cases investigated in this work.

When $\sigma_1^2/\sigma_3^2=10.$, the MINQUE of σ_1^2 yielded the variance almost close to that of BQUE. When σ_1^2/σ_3^2 is 1 or. 1, which is rarely in the practice, the MINQUE of σ_1^2 was sensitive to the a-priori values. However, the robustness could be obtained by eliminating the cases of assigning the a-priori values of σ_1^2/σ_3^2 (the component being estimated is σ_2^2) very small or very large (0. 1 or 10. 0). And the above restriction on the a priori information is not a serious one in the practice.

5. Conclusion

For the 9 layouts investigated the MINQUE is quite robust for all the practical purpoes. AOV adjusted estimator yielded good results except for some ill-structured layouts. Although the caluculations involved in the MINQUE is more laborious than the AOV type estimators, MINQUE gives unified approach in the estimation and since the calculation is almost done by computer (or built-in-packages), MINQUE is recommended. Further investigations on the more general models are recommended.

Referenees

Huh, M.Y. "Robustness of the MINQUE Procedure in Estimating Variance Components", Unpublished Dissertation, Southern Methodist University

(1978).

Low, L.Y., "Sampling Variances of Estimates of Components of Variance from a Non-Orthogonal Two-Way Classification", *Biometvika* (1964), 491～494.

——, "Some Prorerties of Variance Component Estimates in the Two Way Classification," *Technometrics* 18(1976), 39～46.

Rao, C.R., "Estimation of Variance and Covariance Components in Linear Models", *Journal of American Statistical Association* 67 (1972), 112～115.

Appendix

Efficiency Plots for the MINQUE and AOV Estimators of

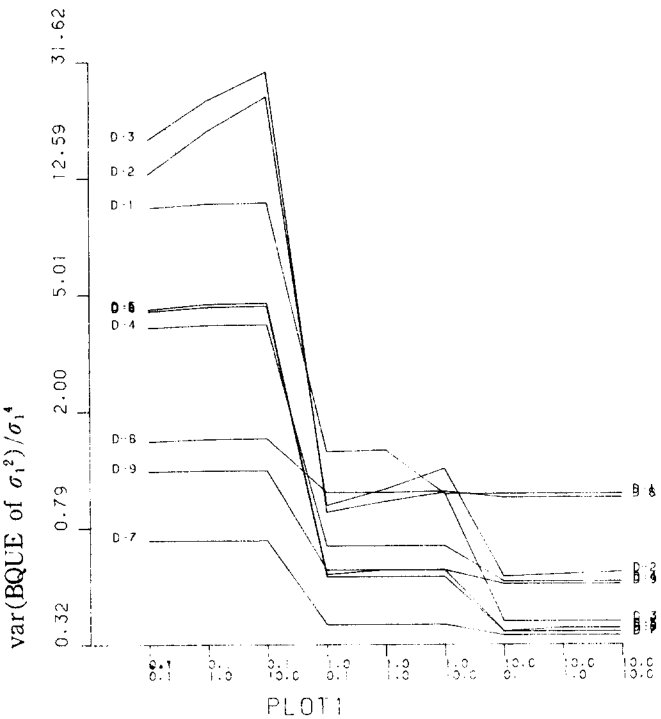
The following 5 plots are selected from the 9 plots. Those not shown here yielded the variances of the MINQUE and AOV estimators very close to the BQUE regardless of the parameter values except for the AOV undjusted extimators. The plots are drawn in the follwing fashion:

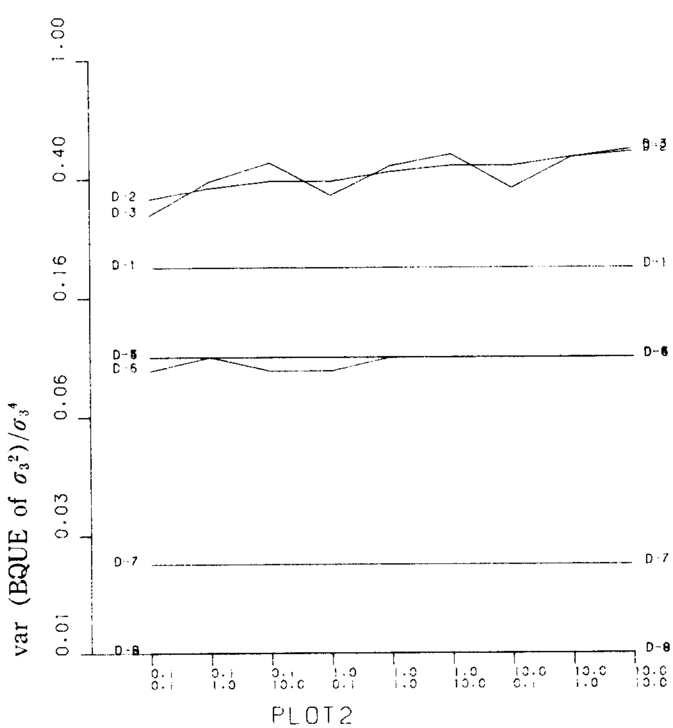
i) The 25 points in the horigontal lines for each plot are concerped with the MINQUE and are in chronlogical order of (ξ_1^2, ξ_2^2) with ξ_2^2 varies first such as The combinations are (0.1, 0.1), (0.1, 0.5), (0.1, 1.0), ..., (10.0, 1.0), (10.0, 2.0), (10.0, 10.0).

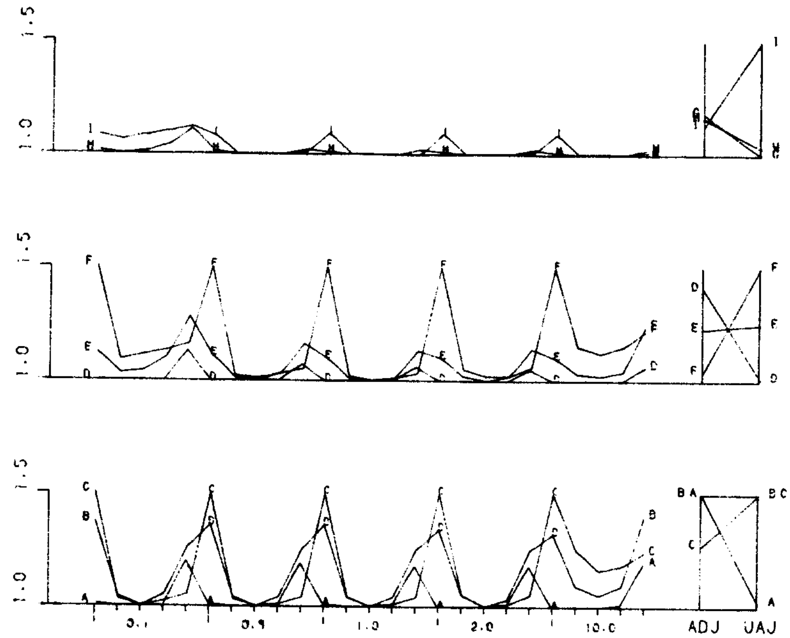
ii) Two added points labeled as ADJ and UAJ stands for the AOV adjusted and AOV unadjusted.

iii) The vertical lines give the efficiency of the estimators, i.e., Variance (relevant estimator of σ_1^2)/variance (BOUE of σ_1^2). Those values exceeding 1.5 are cut to 1.5 for the convenience of the plotting.

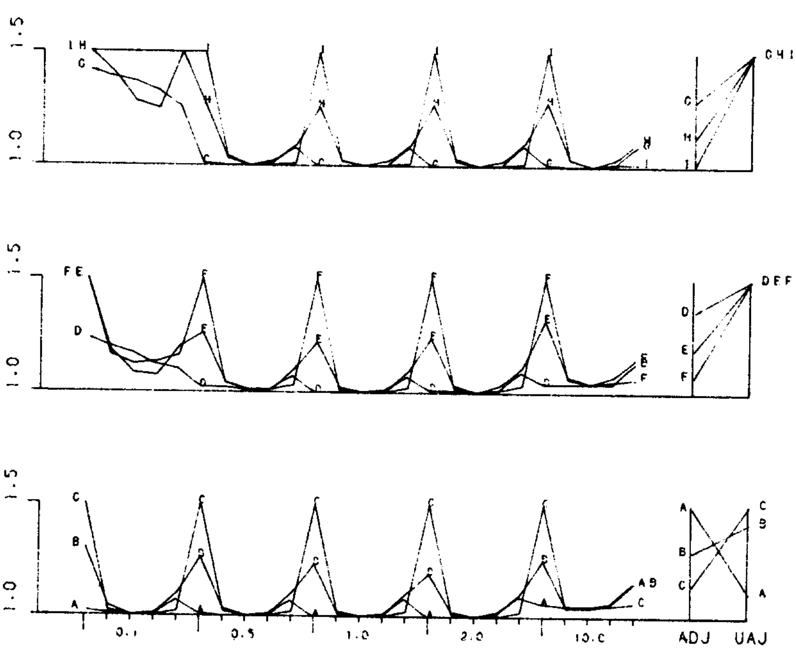
iv) For each plot, there are 3 graphs corresponding to $\rho_2^2=0.1$, 1.0 and 10.0. The alphabets represent the order, i.e., (A,B,C) for $\rho_1^2=0.1$ and $\rho_2^2=(0.1, 1.0, 10.0)$, (D,E,F) for $\rho_1^2=1.0$ and $\rho_2^2=(0.1, 1.0, 10.0)$, (G,H,I) for $\rho_1^2=10.0$ and $\rho_2^2=(0.1, 1.0, 10.0)$


31.62
12.59
5.01
2.00
0.79
0.32
var(BQUE of σ_1^2)/σ_1^4
D-3
D-2
D-1
D-5
D-4
D-6
D-9
D-7
PLOT1

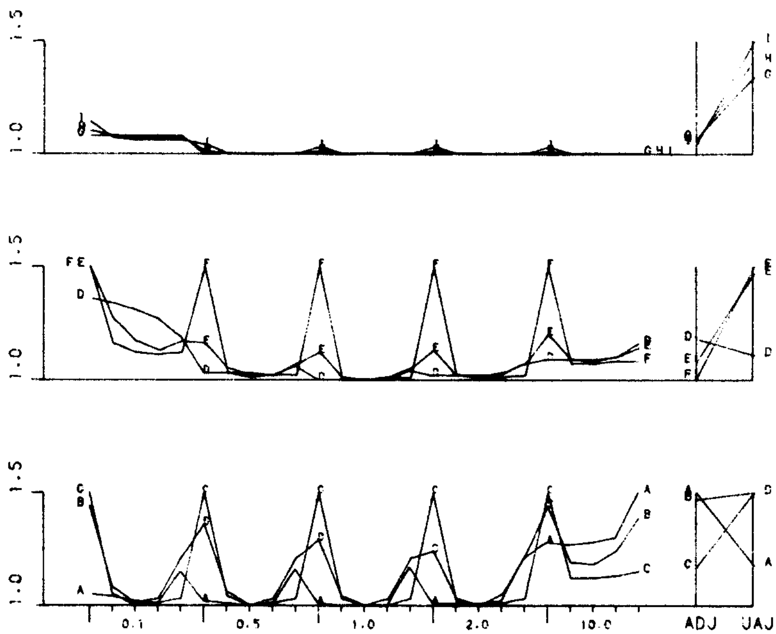

1.00
0.40
0.16
0.06
0.03
0.01
0.0
var (BQUE of σ_3^2)/σ_3^4
D-2
D-3
D-1
D-6
D-7
D-8
PLOT2



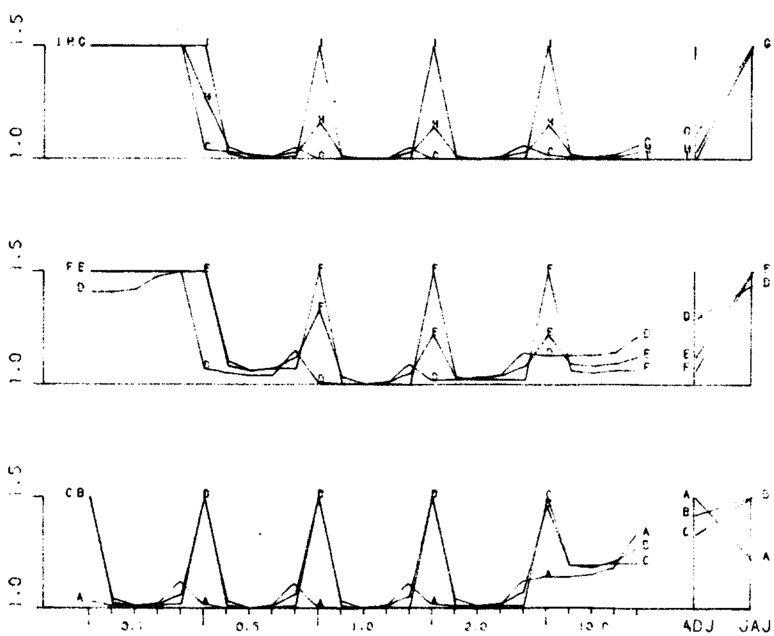
D2-ROW



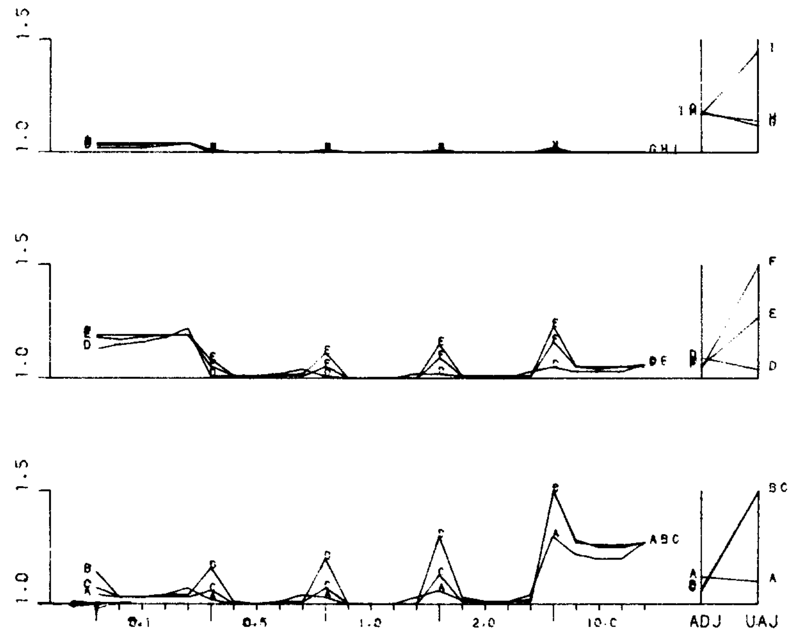
D2-ERROR



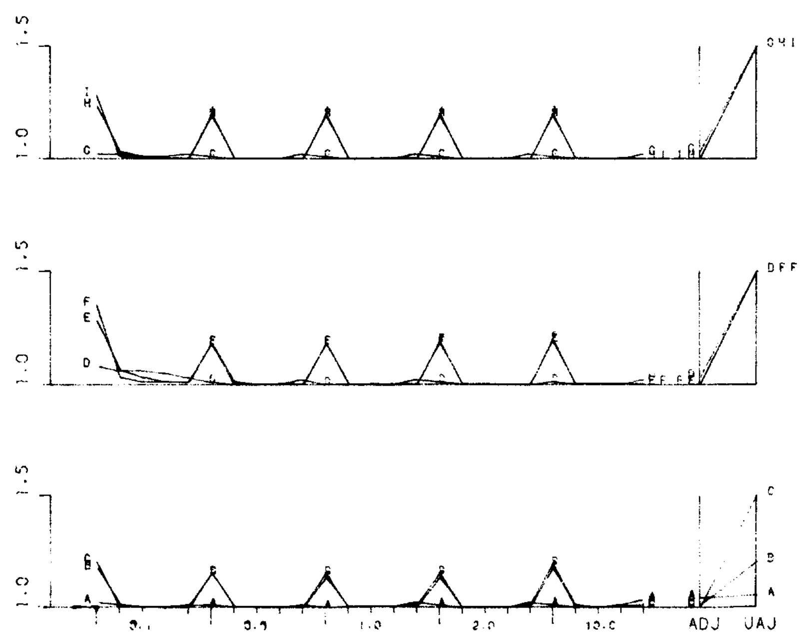
D3-ROW



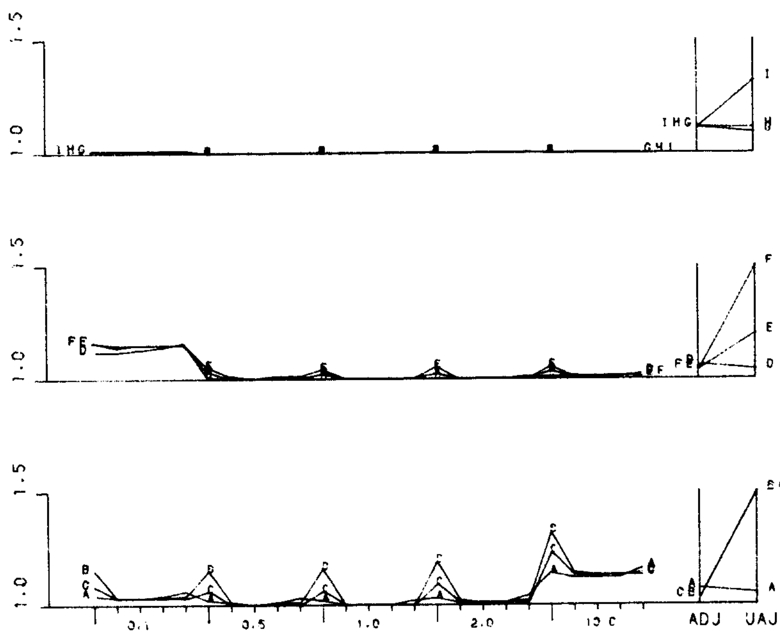
D3-ERROR



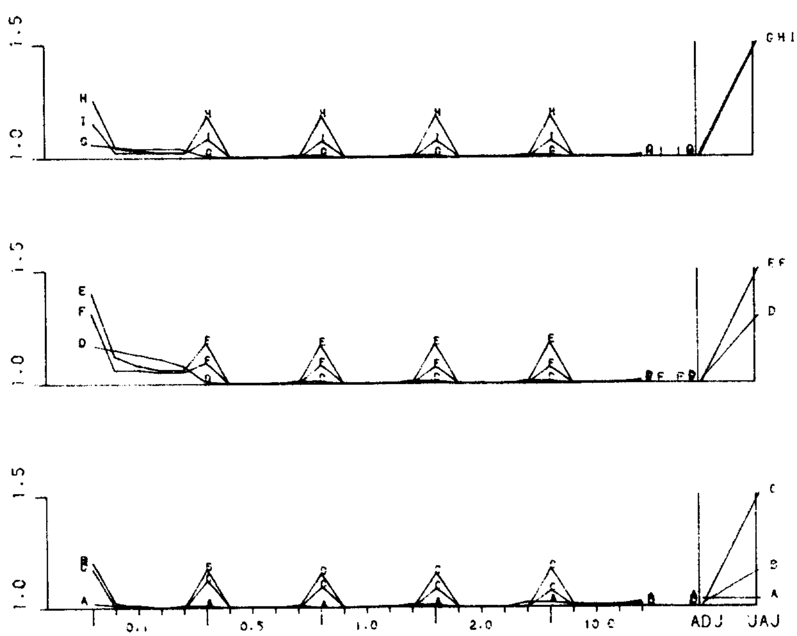
D5-ROW



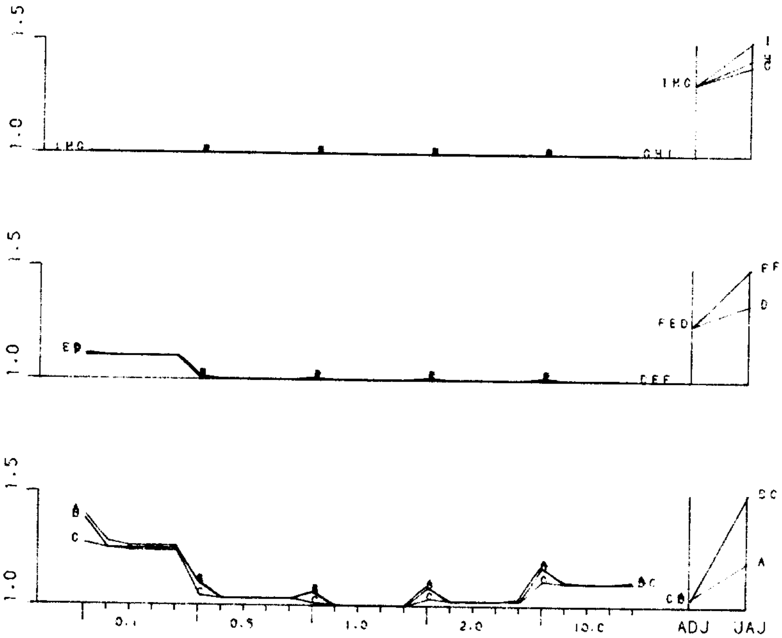
D5-ERROR



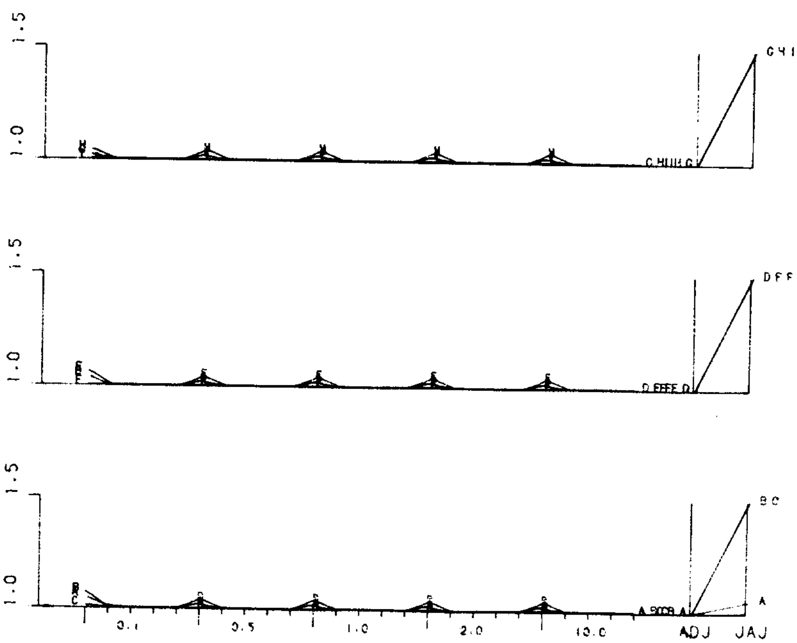
D6-ROW



D6-ERROR



D9-ROW



D9-ERROR