PROOF, AND CORRECTION, OF A RESULT IN A 1961 PAPER ON VARIANCE COMPONENTS

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BU-235-M February, 1967

ABSTRACT

Searle and Henderson (1961, Biometrics 17, 607-616) develop computing procedures for estimating variance components in the 2-way classification, mixed model. The prime object of that paper is presentation of a formula convenient for computing one of the more complicated coefficients that arises in the estimation procedure. Results are given but few details of derivation are shown. These details are now presented, and correction made of an error in the computing formula. The consequences of this correction in the numerical illustration are also given.

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Introduction

The model for the 2-way classification with interaction is

$$x_{ijk} = \mu + \alpha_i + \beta_j + \alpha\beta_{ij} + e_{ijk} \qquad \text{--- (1)}$$

where x_{ijk} is the observation, μ is a general mean, α_i is the effect due to the i'th level of one classification, β_j the effect due to the j'th level of the other classification, $\alpha\beta_{ij}$ the interaction and e_{ijk} the random error term. We suppose that the number of α-classes is a, the number of β-classes is b, and that there are n_{ij} observations in the ij'th subclass, $k = 1,2,\ldots,n_{ij}$ with s subclasses having observations in them, i.e. $n_{ij} \neq 0$ for s subclasses. The uncorrected sum of squares for fitting this model is

$$R(\mu,\alpha,\beta,\alpha\beta) = \sum_{i=1}^{a} \sum_{j=1}^{b} x_{ij.}^2/n_{ij} \qquad \text{--- (2)}$$

where $x_{ij.} = \sum_{k=1}^{n_{ij}} x_{ijk}$.

The model without interaction is

$$x_{ijk} = \mu + \alpha_i + \beta_j + e_{ijk} \, .$$

Suppose θ is the vector containing μ, the α_i's and the β_j's. Then the uncorrected sum of squares for fitting the model can be expressed as

$$R(\mu,\alpha,\beta) = \hat{\theta}w$$

where $\hat{\theta}$ is a solution to the least squares normal equations for fitting this no-interaction model, w being the vector of right-hand sides of these equations. Since $\hat{\theta}$ can be any solution let us take that obtained by putting $\hat{\mu} = 0$ and $\hat{\beta}_b = 0$. Then, writing $\hat{\alpha}' = (\hat{\alpha}_1 \;\; \hat{\alpha}_2 \;\; \ldots \;\; \hat{\alpha}_a)$ and $\hat{\beta}' = (\hat{\beta}_1 \;\; \hat{\beta}_2 \;\; \ldots \;\; \hat{\beta}_{b-1})$ the equations can be written as

$$\begin{bmatrix} P & Q \\ Q' & R \end{bmatrix} \begin{bmatrix} \hat{\alpha} \\ \hat{\beta} \end{bmatrix} = \begin{bmatrix} y \\ z \end{bmatrix} \qquad --- (3)$$

where

$$P = \begin{bmatrix} n_{1.} & & & \\ & n_{2.} & & \\ & & \ddots & \\ & & & n_{a.} \end{bmatrix}, \quad Q = \begin{bmatrix} n_{11} & n_{12} & \cdots & n_{1,b-1} \\ n_{21} & n_{22} & \cdots & n_{2,b-1} \\ \vdots & & & \\ n_{a1} & n_{a2} & \cdots & n_{a,b-1} \end{bmatrix}, \qquad --- (4)$$

$$R = \begin{bmatrix} n_{.1} & & & \\ & n_{.2} & & \\ & & \ddots & \\ & & & n_{.b-1} \end{bmatrix}, \quad y = \begin{bmatrix} x_{1..} \\ x_{2..} \\ \vdots \\ x_{a..} \end{bmatrix} \text{ and } z = \begin{bmatrix} x_{.1.} \\ x_{.2.} \\ \vdots \\ x_{.b-1} \end{bmatrix}.$$

Q, R and z' have b-1 columns because of taking $\hat{\beta}_b = 0$. In this way

$$R(\mu,\alpha,\beta) = (\hat{\alpha}', \; \hat{\beta}') \begin{bmatrix} y \\ z \end{bmatrix} = (y' \;\; z') \begin{bmatrix} P & Q \\ Q & R \end{bmatrix}^{-1} \begin{bmatrix} y \\ z \end{bmatrix}, \qquad --- (5)$$

which is equation (8) of the 1961 paper.

The situation considered in that paper is the interaction model with one classification fixed and the other random, namely the mixed model with interaction. In particular the α-effects are taken as random having zero means and variance-covariance matrix $\sigma^2_{\alpha} I_a$, and the β-effects are taken as fixed; the interaction terms are also taken as random effects, having zero means and variance-covariance matrix $\sigma^2_{\alpha\beta} I$. The error terms are, of course, random, with zero means and variances σ_e^2; and all random terms, the α's, the $\alpha\beta$'s and the e's, are uncorrelated with themselves and each other. In this context the 1961 paper is concerned with deriving estimates of σ_α^2, $\sigma_{\alpha\beta}^2$ and σ_e^2 by the method of equating differences between sums of squares to their expectations. And one term used in this manner is, for E denoting expectation,

$$E[R(\mu,\alpha,\beta,\alpha\beta) - R(\mu,\alpha,\beta)] = (N - k_\beta)\sigma_{\alpha\beta}^2 + (s - a - b + 1)\sigma_e^2 \quad --- (6)$$

where k_β is given as

$$k_\beta = 2\mathrm{tr}(AU + 2BV + DW) \quad --- (7)$$

with $N = n_{..} = \sum_{i=1}^{a} \sum_{j=1}^{b} n_{ij}$. These results are correct, but an error in the published definition of U leads to incorrect computing formulae for k_β. The correction is easy, it merely involves changing an upper limit of summation from b-1 to b, but since the published paper contains no details for deriving (6) and (7) the error is not only corrected here but validation is given also.

<u>Expansion of $R(\mu,\alpha,\beta)$</u>

Suppose that $\begin{bmatrix} P & Q \\ Q' & R \end{bmatrix}^{-1} = \begin{bmatrix} A & B \\ B' & D \end{bmatrix}$ --- (8)

Then from (5)

$$R(\mu,\alpha,\beta) = y'Ay + 2y'Bz + z'Dz$$

$$= \mathrm{tr}(Ayy' + 2Bzy' + Dqq') \quad --- (9)$$

where tr represents the operation of taking the trace of a matrix. Furthermore, from (8)

$$A = P^{-1} + P^{-1}QDQ'P^{-1} ,$$

$$B = -P^{-1}QD , \quad --- (10)$$

and $$D = (R - Q'P^{-1}Q)^{-1} .$$

Expressions for y and z

In order to find the expected value of (9) for use in (6) we first establish matrix expressions for y and z on the basis of the model (1). With the β_j-effects fixed μ can be absorbed into the β_j's by writing

$$\gamma_j = \mu + \beta_j$$

so that the model becomes

$$x_{ijk} = \alpha_i + \gamma_j + (\alpha\beta)_{ij} + e_{ijk} \quad\quad --- (11)$$

Then

$$y = \begin{bmatrix} x_{1..} \\ x_{2..} \\ \vdots \\ x_{a..} \end{bmatrix}$$

$$= \begin{bmatrix} n_{1.} & \cdot & \cdots & \\ \cdot & n_{2.} & & \\ & & \ddots & \\ \cdot & \cdot & & n_{a.} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_a \end{bmatrix} + \begin{bmatrix} n_{11} & n_{12} & \cdots & n_{1b} \\ n_{21} & n_{22} & \cdots & n_{2b} \\ & & & \\ n_{a1} & n_{a2} & \cdots & n_{ab} \end{bmatrix} \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_b \end{bmatrix}$$

$$+ \begin{bmatrix} n_{11} \; n_{12} \cdots n_{1b} & & & \\ & n_{21} \cdots n_{2b} & & \\ & & \ddots & \\ & & & n_{a1} \; n_{a2} \cdots n_{ab} \end{bmatrix} \begin{bmatrix} \alpha\beta_{11} \\ \alpha\beta_{12} \\ \vdots \\ \alpha\beta_{1b} \\ \vdots \\ \alpha\beta_{a1} \\ \alpha\beta_{a2} \\ \vdots \\ \alpha\beta_{ab} \end{bmatrix}$$

$$+ (\bar{e}_{1.} \quad \bar{e}_{2.} \quad \cdots \quad \bar{e}_{a.})' \; ;$$

and

$$z = \begin{bmatrix} \bar{x}_{.1.} \\ \bar{x}_{.2.} \\ \vdots \\ \bar{x}_{.,b-1,.} \end{bmatrix}$$

$$= \begin{bmatrix} n_{11} & n_{21} & \cdots & n_{a1} \\ n_{12} & n_{22} & \cdots & n_{a2} \\ \vdots & & & \\ n_{1,b-1} & n_{2,b-1} & \cdots & n_{a,b-1} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_a \end{bmatrix} + \begin{bmatrix} n_{.1} & & & \\ & n_{.2} & & \\ & & \ddots & \\ & & & n_{1,b-1} \end{bmatrix} \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_{b-1} \end{bmatrix}$$

$$+ \begin{bmatrix} n_{11} \cdot \cdots \cdot & 0 & n_{21} \cdot \cdots \cdot & 0 & \cdots & n_{a1} \cdot \cdots \cdot & 0 \\ n_{12} & 0 & n_{22} & 0 & & n_{a2} & 0 \\ \ddots & \vdots & \ddots & \vdots & & \ddots & \vdots \\ n_{1,b-1} & 0 & n_{2,b-1} & 0 & & n_{a,b-1} & 0 \end{bmatrix} \begin{bmatrix} \alpha\beta_{11} \\ \alpha\beta_{12} \\ \vdots \\ \alpha\beta_{1b} \\ \alpha\beta_{21} \\ \vdots \\ \alpha\beta_{2b} \\ \vdots \\ \alpha\beta_{a1} \\ \vdots \\ \alpha\beta_{ab} \end{bmatrix}$$

$$+ (\bar{e}_{.1.} \quad \bar{e}_{.2.} \quad \cdots \quad \bar{e}_{.,b-1,.})' \ .$$

To write these expressions more simply we define the following matrices and vectors:

$$S = \begin{bmatrix} n_{11} & n_{12} & \cdots & n_{1b} & & & & & & & & \\ & & & & n_{21} & n_{22} & \cdots & n_{2b} & & & & \\ & & & & & & & & \ddots & & & \\ & & & & & & & & & n_{a1} & n_{a2} & \cdots & n_{ab} \end{bmatrix}$$

$$T = \begin{bmatrix} n_{11} & & & 0 & n_{21} & & & 0 & \cdots & n_{a1} & & & 0 \\ & n_{12} & & 0 & & n_{22} & & 0 & & & n_{a2} & & 0 \\ & & \ddots & \vdots & & & \ddots & \vdots & & & & \ddots & \vdots \\ & & n_{1,b-1} & 0 & & & n_{2,b-1} & 0 & & & & n_{a,b-1} & 0 \end{bmatrix} \qquad \text{--- (12)}$$

$\gamma' = (\gamma_1 \quad \gamma_2 \quad \cdots \quad \gamma_{b-1})$, the vector of $\mu+\beta_j$ terms, of order b-1 ;

ϵ' = the vector of $\alpha\beta$ terms, of order ab ,

e_y = the vector of $\bar{e}_{i..}$ terms in y, of order a ,

e_z = the vector of $\bar{e}_{.j.}$ terms in z, of order b-1 ,

and

$n_b' = (n_{1b} \quad n_{2b} \quad \cdots \quad n_{ab})$.

With these definitions and using P, Q and R given earlier

$$y = P\alpha + (Q \quad n_b) \begin{bmatrix} \gamma \\ \gamma_b \end{bmatrix} + S\epsilon + e_y \qquad \text{--- (13)}$$

and $z = Q'\alpha + R\gamma + T\epsilon + e_z$. --- (14)

Expected values

To establish (6) we first require $ER(\mu,\alpha,\beta,\alpha\beta)$, which is easily obtained. Substituting (11) into (2) gives

$$R(\mu,\alpha,\beta,\alpha\beta) = \sum_{i=1}^{a}\sum_{j=1}^{b} \frac{(n_{ij}\alpha_i + n_{ij}\gamma_j + n_{ij}\alpha\beta_{ij} + e_{ij.})^2}{n_{ij}}$$

and on taking expectations in accord with the model this gives

$$ER(\mu,\alpha,\beta,\alpha\beta) = N\sigma^2_\alpha + \sum_{j=1}^{b} n_{.j}\gamma_j^2 + N\sigma^2_{\alpha\beta} + s\sigma^2_e . \qquad --- (15)$$

Derivation of $ER(\mu,\alpha,\beta)$ is more complex. It is achieved by noting from (9) that

$$ER(\mu,\alpha,\beta) = tr[AE(yy') + 2BE(zy') + DE(zz')] \qquad --- (16)$$

and into this substituting y and z from (13) and (14). We take each term of (16) in turn. Thus

$$trAE(yy') = trAE\left[P\alpha+(Q \quad n_b)\begin{pmatrix}\gamma\\ \gamma_b\end{pmatrix} + S\epsilon + e_y\right]\left[\alpha'P'+(\gamma' \quad \gamma_b)\begin{pmatrix}Q'\\ n_b\end{pmatrix} + \epsilon'S' + e_y'\right]$$

$$= trA\left[PE(\alpha\alpha')P'+(Q \quad n_b)E\begin{pmatrix}\gamma\gamma' & \gamma\gamma_b\\ \gamma_b\gamma' & \gamma_b\gamma_b'\end{pmatrix}\begin{pmatrix}Q'\\ n_b\end{pmatrix} + SE(\epsilon\epsilon')S' + E(e_y e_y')\right]$$

$$= trA[PP'\sigma^2_\alpha + Q^*E(\gamma^*\gamma^{*\prime})Q^{*\prime} + SS'\sigma^2_{\alpha\beta} + P\sigma^2_e]$$

where $Q^* = (Q \quad n_b)$ and $\gamma^{*\prime} = (\gamma' \quad \gamma_b)$.

Hence

$$trAE(yy') = \sigma^2_\alpha tr(APP') + tr[AQ^*E(\gamma^*\gamma^{*\prime})Q^{*\prime}] + \sigma^2_{\alpha\beta}tr(ASS') + \sigma^2_e tr(AP). \quad -- (17)$$

Similarly, the second term in (16) is, from (13) and (14),

$$2trBE(zy') = 2trB(Q'\alpha + R\gamma + T\epsilon + e_z)(\alpha'P' + \gamma^{*\prime}Q^{*\prime} + \epsilon'S' + e_y')$$

$$= 2trB[Q'P'\sigma^2_\alpha + RE(\gamma\gamma^{*\prime})Q^{*\prime} + TS'\sigma^2_{\alpha\beta} + Q\sigma^2_e]$$

$$= 2\sigma^2_\alpha tr(BQ'P') + 2trBRE(\gamma\gamma^{*\prime})Q^{*\prime} + 2\sigma^2_{\alpha\beta}tr(BTS') + 2\sigma^2_e tr(BQ). \quad - (18)$$

Likewise the third term is

$$\begin{aligned} \mathrm{trDE}(zz') &= \mathrm{trDE}(Q'\alpha + R\gamma + T\epsilon + e_z)(\alpha' Q + \gamma' R' + \epsilon' T' + e_z') \\ &= \mathrm{trD}[Q'Q\sigma^2_\alpha + RE(\gamma\gamma')R' + TT'\sigma^2_{\alpha\beta} + R\sigma^2_e] \\ &= \sigma^2_\alpha \mathrm{tr}(DQ'Q) + \mathrm{trDRE}(\gamma\gamma')R' + \sigma^2_{\alpha\beta}\mathrm{tr}(DTT') + \sigma^2_e \mathrm{tr}(DR) . \quad --- (19) \end{aligned}$$

Combining (17), (18) and (19) in (16) gives

$$\begin{aligned} ER(\mu,\alpha,\beta) &= \sigma^2_\alpha \mathrm{tr}(APP' + 2BQ'P' + DQ'Q) \\ &+ \mathrm{tr}[AQ^*E(\gamma^*\gamma^{*\prime})Q^{*\prime} + 2BRE(\gamma\gamma^{*\prime})Q^{*\prime} + DRE(\gamma\gamma')R'] \\ &+ \sigma^2_{\alpha\beta}\mathrm{tr}(ASS' + 2BTS' + DTT') + \sigma^2_e \mathrm{tr}(AP + BQ + DR) \quad --- (20) \end{aligned}$$

Taking each of these terms in turn and utilizing both the definitions of the matrices involved, especially (10), and the cyclic commutative property of matrix products under the trace operation, we find firstly that

$$\begin{aligned} \sigma^2_\alpha \mathrm{tr}(APP' + 2BQ'P' + DQ'Q) &= \sigma^2_\alpha \mathrm{tr}(PAP + 2Q'PB + Q'QD) \\ &= \sigma^2_\alpha \mathrm{tr}(P + QDQ' - 2Q'QD + Q'QD) \quad \text{from (10)} \\ &= \sigma^2_\alpha \mathrm{tr}(P) \\ &= N\sigma^2_\alpha . \quad --- (21) \end{aligned}$$

In the second term of (20) the γ's are fixed effects, and after substituting for γ^* and Q^* the term becomes

$$\mathrm{tr}\left[\begin{pmatrix} \gamma \\ \gamma_b \end{pmatrix} (\gamma' \quad \gamma_b) \begin{pmatrix} Q' \\ n_b' \end{pmatrix} A(Q \quad n_b) + 2\gamma(\gamma' \quad \gamma_b) \begin{pmatrix} Q' \\ n_b' \end{pmatrix} BR + \gamma\gamma' RDR \right]$$

$$\begin{aligned} &= (\gamma' Q' + \gamma_b n_b')A(Q\gamma + n_b\gamma_b) + 2(\gamma' Q' + \gamma_b n_b')BR\gamma + \gamma' RDR\gamma \\ &= \gamma'(Q'AQ + 2Q'BR + RDR)\gamma + \gamma_b n_b'(2AQ\gamma + \gamma_b A n_b + 2BR\gamma) \\ &= \gamma'[Q'(AQ + BR) + (Q'B + RD)R]\gamma + \gamma_b n_b'[2(AQ + BR)\gamma + \gamma_b A n_b] \\ &= \gamma'[Q'(0) + (I)R]\gamma + \gamma_b n_b'[2(0)\gamma + \gamma_b A n_b] \quad \text{from (10)} \\ &= \gamma' R\gamma + \gamma_b^2 n_b' A n_b . \quad --- (22) \end{aligned}$$

Now consider the determinant

$$\begin{vmatrix} P & Q & n_b \\ Q' & R & 0 \\ n_b' & 0 & n_{.b} \end{vmatrix} .$$

By the definition of its elements its value is zero. As an example, suppose the numbers of observations are as shown in Table 1 (the example of the earlier paper).

(Show Table 1)

Then the value of the above determinant for this example is

$$\left|\begin{array}{ccccc|ccc|c} 10 & \cdot & \cdot & \cdot & \cdot & 1 & 2 & 3 & 4 \\ \cdot & 20 & \cdot & \cdot & \cdot & 3 & 6 & 4 & 7 \\ \cdot & \cdot & 40 & \cdot & \cdot & 12 & \cdot & 12 & 16 \\ \cdot & \cdot & \cdot & 50 & \cdot & 12 & 12 & 13 & 13 \\ \cdot & \cdot & \cdot & \cdot & 50 & 25 & 25 & \cdot & \cdot \\ \hline 1 & 3 & 12 & 12 & 25 & 53 & \cdot & \cdot & \cdot \\ 2 & 6 & \cdot & 12 & 25 & \cdot & 45 & \cdot & \cdot \\ 3 & 4 & 12 & 13 & \cdot & \cdot & \cdot & 32 & \cdot \\ \hline 4 & 7 & 16 & 13 & \cdot & \cdot & \cdot & \cdot & 40 \end{array}\right|$$

which is clearly zero (its last 4 rows have the same sum as do the first 5 rows). And in general

$$\begin{vmatrix} P & Q & n_b \\ Q' & R & 0 \\ n_b' & 0 & n_{.b} \end{vmatrix} = 0 .$$

Expanding the left-hand side, partitioned before the last row and column, gives

$$\begin{vmatrix} P & Q \\ Q' & R \end{vmatrix} \left| n_{.b} - (n_b' \quad 0) \begin{bmatrix} P & Q \\ Q' & R \end{bmatrix}^{-1} \begin{bmatrix} n_b \\ \ \end{bmatrix} \right| = 0$$

and because $\begin{vmatrix} P & Q \\ Q' & R \end{vmatrix} \neq 0$ this means

$$n_{.b} = (n_b' \quad 0) \begin{bmatrix} P & Q \\ Q' & R \end{bmatrix}^{-1} \begin{bmatrix} n_b \\ 0 \end{bmatrix}$$

$$= (n_b' \quad 0) \begin{bmatrix} A & B \\ B & D \end{bmatrix} \begin{bmatrix} n_b \\ 0 \end{bmatrix}$$

$$= n_b' A n_b \ .$$

Substituting this and the definition of R shown in (4) into (22) gives the second term of (20) as

$$\gamma' R \gamma + n_{.b}\gamma_b^2 = \sum_{j=1}^{b} n_{.j}\gamma_j^2 \ . \qquad --- (23)$$

And the last term in (20) is

$$\begin{aligned} \sigma_e^2 \mathrm{tr}(AP + 2BQ + DR) &= \sigma_e^2 \mathrm{tr}(I_a + P^{-1}QDQ' - 2P^{-1}QDQ' + DR) \\ &= \sigma_e^2 \mathrm{tr}(I_a + DR - Q'P^{-1}QD) \\ &= \sigma_e^2 \mathrm{tr}(I_a + I_{b-1}) \\ &= (a + b - 1)\sigma_e^2 \ . \qquad --- (24) \end{aligned}$$

And now, putting (21), (23) and (24) into (20) gives

$$ER(\mu,\alpha,\beta) = N\sigma_\alpha^2 + \sum_{j=1}^{b} n_{.j}\gamma_j^2 + \sigma_{\alpha\beta}^2 \mathrm{tr}(ASS' + 2BTS' + DTT') + (a + b - 1)\sigma_e^2 \ ,$$

and subtracting this from (15) gives

$$E[R(\mu,\alpha,\beta,\alpha\beta) - R(\mu,\alpha,\beta)] = [N - \mathrm{tr}(ASS'+2BTS'+DTT')]\sigma_{\alpha\beta}^2 + (s-a-b+1)\sigma_e^2$$

which is exactly the form of (6) with

$$k_\beta = \mathrm{tr}(ASS' + 2BTS' + DTT') \ . \qquad --- (25)$$

In comparison to (7) a typographical error of the 1961 paper is immediately apparent: there should be no "2" multiplying the trace expression for k_β; i.e. expression (25) is correct, without doubling its right-hand side.

If k_β is now written in the same form as the '61 paper (omitting the erroneous 2),

$$k_\beta = tr(AU + 2BV + DW) ,$$

and comparison of this with (25) defines U, V and W. Thus U = SS', a diagonal matrix of order a, with elements $\sum_{j=1}^{b} n_{ij}^2$ for i = 1,2,...,a . Here lies the major error in the 1961 paper; the elements of U are there defined as $\sum_{j=1}^{b-1} n_{ij}^2$ whereas, as just shown, they are $\sum_{j=1}^{b} n_{ij}^2$, the upper limit of the summation being b and not b-1. Similarly

$$V = TS' = \{v_{ji} = n_{ij}^2\} \text{ for } j = 1,2,\ldots,b\text{-}1 \text{ and } i = 1,2,\ldots,a,$$

a matrix of order b-1 by a with elements n_{ij}^2 .

Here is a relatively obvious error in the '61 paper: V is there defined as having order a by b-1; it is, as just demonstrated, b-1 X a. And finally, as correctly defined in the published paper

W = TT' is a diagonal matrix of order b-1, with elements

$$\sum_{i=1}^{a} n_{ij}^2 \text{ for } j = 1,2,\ldots,b\text{-}1 .$$

<u>Summary for k_β</u>

In the notation of the 1961 paper

$$E[R(\mu,\alpha,\beta,\alpha\beta) - R(\mu,\alpha,\beta)] = (n_{..} - k_\beta)\sigma_{\alpha\beta}^2 + (s - a - b + 1)\sigma_e^2$$

with

$$k_\beta = tr(AU + 2BV + DW)$$

where the normal equations for fitting the no-interaction model (with $\hat{\mu} = 0$ and $\hat{\beta}_b = 0$) have matrix of coefficients

$$\begin{bmatrix} P & Q \\ Q' & R \end{bmatrix} = \left[\begin{array}{ccc|ccc} n_{1.} & & & n_{11} & \cdots & n_{1,b-1} \\ & \ddots & & \vdots & & \\ & & n_{a.} & n_{a1} & \cdots & n_{a,b-1} \\ \hline n_{..} & \cdots & n_{a1} & n_{.1} & & \\ \vdots & & \vdots & & \ddots & \\ n_{1,b-1} & & n_{a,b-1} & & & n_{.,b-1} \end{array}\right] ,$$

where $$\begin{bmatrix} P & Q \\ Q' & R \end{bmatrix}^{-1} = \begin{bmatrix} A & B \\ B' & D \end{bmatrix}$$

and $$\begin{bmatrix} U & V' \\ V & W \end{bmatrix} = \left[\begin{array}{ccc|ccc} \sum_{j=1}^{b} n_{1j}^2 & & & n_{11}^2 & \cdots & n_{1,b-1}^2 \\ & \ddots & & \vdots & & \vdots \\ & & \sum_{j=1}^{b} n_{aj}^2 & n_{a1}^2 & \cdots & n_{a,b-1}^2 \\ \hline n_{11}^2 & \cdots & n_{a1}^2 & \sum_{i=1}^{a} n_{i1}^2 & & \\ \vdots & & \vdots & & \ddots & \\ n_{1,b-1}^2 & \cdots & n_{a,b-1}^2 & & & \sum_{i=1}^{a} n_{i,b-1}^2 \end{array}\right] .$$

Computing formulae

The calculation of k_β as summarized above presents no problem conceptually: simply invert a matrix to obtain A, B and D and use these matrices to calculate k_β as

$$k_\beta = \text{tr} \begin{bmatrix} A & B \\ B' & D \end{bmatrix} \begin{bmatrix} U & V' \\ V & W \end{bmatrix} .$$

However, in applications where a and/or b are very large, some hundreds maybe, the inversion to derive A, B and D might be troublesome – even on to-day's large computers. However, if b is very small compared to a the partitioned form of the inverse given in (10) should be used, for it involves inverting a matrix of order b-1 rather than one of order a+b-1 . [An advantageous use of this technique is given in Searle and Henderson (1960) where a = 600 and b =5.] Furthermore, using this partitioned inverse leads to a more explicit computing formula for k_β. Thus from (10), for

$$C = R - Q'P^{-1}Q$$

the elements of C are

$$c_{jj} = n_{.j} - \sum_{i=1}^{a} \frac{n_{ij}^2}{n_{i.}} \quad \text{for } j = 1,2,\ldots,b-1 \; ,$$

and $$c_{jj'} = - \sum_{i=1}^{a} \frac{n_{ij}n_{ij'}}{n_{i.}} \quad \text{for } j \neq j' = 1,2,\ldots,b-1 \; .$$

And on computing c_{bj} an arithmetic check is provided, namely that for all j $\sum_{j'=1}^{b} c_{jj'} = 0$. Thus the matric C can be readily obtained, and its inverse, C^{-1}, is D. Denoting the elements of this inverse by $d_{jj'}$ for $j,j' = 1,2,\ldots,b-1$, we then have

$$B = -P^{-1}QD = \{b_{ij}\}$$

with $$b_{ij} = - \frac{1}{n_{i.}} \sum_{q=1}^{b-1} n_{iq}d_{qj} \; , \quad \text{for } i = 1,2,\ldots,a \text{ and } j = 1,2,\ldots,b-1 \; .$$

And

$$A = P^{-1} + P^{-1}QDQ'P^{-1} = \{a_{ii'}\}$$

with $$a_{ii} = \frac{1}{n_{i.}} + \sum_{s=1}^{b-1} (-b) \frac{n_{is}}{n_{i.}}$$

$$= \frac{1}{n_{i.}} + \frac{1}{n_{i.}^2} \sum_{s=1}^{b-1} \sum_{q=1}^{b-1} n_{is}n_{iq}d_{qs} \; , \quad \text{for } i = 1,2,\ldots,a \; .$$

In this way

$$k_\beta = tr(AU + 2BV + DW)$$

$$= \sum_{i=1}^{a} a_{ii}u_{ii} + 2 \sum_{i=1}^{a} \sum_{j=1}^{b-1} b_{ij}v_{ji} + \sum_{j=1}^{b-1} d_{jj}w_{jj}$$

$$= \sum_{i=1}^{a} \left[\frac{1}{n_{i.}} + \frac{1}{n_{i.}^2} \sum_{s=1}^{b-1} \sum_{q=1}^{b-1} n_{is}n_{iq}d_{qs} \right] \left[\sum_{j=1}^{b} n_{ij}^2 \right]$$

$$- 2 \sum_{i=1}^{a} \sum_{j=1}^{b-1} \frac{1}{n_{i.}} \sum_{q=1}^{b-1} n_{iq} d_{qj} n_{ij}^2 + \sum_{j=1}^{b-1} d_{jj} \sum_{i=1}^{a} n_{ij}^2$$

$$= \sum_{i=1}^{a} \frac{\sum_{j=1}^{b} n_{ij}^2}{n_{i.}} + \sum_{s=1}^{b-1} \sum_{q=1}^{b-1} d_{qs} \sum_{i=1}^{a} \left\{ \frac{n_{is} n_{iq} \left(\sum_{j=1}^{b} n_{ij}^2 \right)}{n_{i.}^2} - 2 \frac{n_{iq} n_{is}^2}{n_{i.}} \right\}$$

$$+ \sum_{j=1}^{b-1} d_{jj} \sum_{j=1}^{a} n_{ij}^2$$

$$= \sum_{j=1}^{a} \frac{\sum_{j=1}^{b} n_{ij}^2}{n_{i.}} + \sum_{q=1}^{b-1} d_{qq} \sum_{i=1}^{a} \left\{ \frac{n_{iq}^2 \left(\sum_{j=1}^{b} n_{ij}^2 \right)}{n_{i.}^2} - \frac{2n_{iq}^3}{n_{i.}} + n_{iq}^2 \right\}$$

$$+ 2 \sum_{s>q=1}^{b-1} \sum d_{qs} \sum_{i=1}^{a} \left\{ \frac{n_{is} n_{iq} \left(\sum_{j=1}^{b} n_{ij}^2 \right)}{n_{i.}^2} - \frac{n_{is} n_{iq}^2}{n_{i.}} - \frac{n_{is}^2 n_{iq}}{n_{i.}} \right\}$$

$$= \sum_{i=1}^{a} \frac{\sum_{j=1}^{b} n_{ij}^2}{n_{i.}} + \sum_{q=1}^{b-1} d_{qq} \sum_{i=1}^{a} \frac{n_{iq}^2}{n_{i.}} \left\{ \frac{\sum_{j=1}^{b} n_{ij}^2}{n_{i.}} - 2n_{iq} + n_{i.} \right\}$$

$$+ 2 \sum_{s>q=1}^{b-1} \sum d_{qs} \sum_{i=1}^{a} \frac{n_{is} n_{iq}}{n_{i.}} \left\{ \frac{\sum_{j=1}^{b} n_{ij}^2}{n_{i.}} - n_{iq} - n_{is} \right\} .$$

With

$$\lambda_i = \sum_{j=1}^{b} \frac{n_{ij}^2}{n_{i.}} \qquad \text{--- (26)}$$

$$f_{i,jj} = \frac{n_{ij}^2}{n_{i.}} (\lambda_i + n_{i.} - 2n_{ij}), \text{ for } j = 1,2,\ldots,b \qquad \text{--- (27)}$$

and

$$f_{i,jj'} = \frac{n_{ij}n_{ij'}}{n_{i.}} (\lambda_i - n_{ij} - n_{ij'}), \text{ for } j \neq j' = 1,2,\ldots,b \qquad --- (28)$$

the expression for k_β becomes

$$k_\beta = \sum_{i=1}^{a} \lambda_i + \sum_{j=1}^{b-1} d_{jj} \left(\sum_{i=1}^{a} f_{i,jj} \right) + 2 \sum_{j'>j}^{b-1} \sum d_{jj'} (f_{i,jj'}) \; . \qquad --- (29)$$

There are two corrections here compared to the corresponding expression in the '61 paper: the upper limit of summation in λ_i is b and not b-1, and in the last term of k_β the summation is for $j' > j$ and not for $j' \neq j$; (or alternatively it is for $j' \neq j$ but not preceded by a factor of 2). With the correction in λ_i comes an alteration in the check that can be used in calculating the f's:

$$\sum_{j'=1}^{b} f_{i,jj'} = f_{i,jj'} + \sum_{\substack{j'=1 \\ j'\neq j}}^{b} f_{i,jj'}$$

$$= \frac{n_{ij}^2}{n_{i.}} (\lambda_i + n_{i.} - 2n_{ij}) + \frac{n_{ij}(\lambda_i - n_{ij})}{n_{i.}} \sum_{\substack{j'=1 \\ j'\neq j}}^{b} n_{ij'} - \frac{n_{ij}}{n_{i.}} \sum_{\substack{j'=1 \\ j'\neq j}}^{b} n_{ij}^2$$

$$= \frac{n_{ij}^2}{n_{i.}} (\lambda_i + n_{i.} - 2n_{ij}) + \frac{n_{ij}(\lambda_i - n_{ij})(n_{i.} - n_{ij})}{n_{i.}} - \frac{n_{ij}(n_{i.}\lambda_i - n_{ij}^2)}{n_{i.}}$$

$$= (n_{ij}/n_{i.})[n_{ij}(\lambda_i + n_{i.} - 2n_{ij}) + n_{ij}(-\lambda_i - n_{i.} + n_{ij} + n_{ij})] \; ; \qquad --- (30)$$

i.e. $\sum_{j=1}^{b} f_{i,jj'} = 0$.

This condition replaces equation (1͏̈) of the 1961 paper.

Example

As already indicated the hypothetical example in the published paper is that shown in Table 1. From this it can be seen that the detailed calculations of λ_1 and the $f_{1,jj'}$'s, based on (26), (27), and (28) are as follows:

$$\begin{aligned}
\lambda_1 &= (1^2 + 2^2 + 3^2 + 4^2)/10 = 3.0 \\
f_{1,11} &= (1^2/10)(3 + 10 - 2) = 1.1 \\
f_{1,22} &= (2^2/10)(3 + 10 - 4) = 3.6 \\
f_{1,33} &= (3^2/10)(3 + 10 - 6) = 6.3 \\
f_{1,44} &= (4^2/10)(3 + 10 - 8) = 8.0 \\
f_{1,12} &= (2/10)(3 - 1 - 2) = 0.0 \\
f_{1,13} &= (3/10)(3 - 1 - 3) = -0.3 \\
f_{1,14} &= (4/10)(3 - 1 - 4) = -0.8 \\
f_{1,23} &= (6/10)(3 - 2 - 3) = -1.2 \\
f_{1,24} &= (8/10)(3 - 2 - 4) = -2.4 \\
f_{1,34} &= (12/10)(3 - 3 - 4) = -4.8 .
\end{aligned}$$

The differences between these and the published values arise solely from the corrected value of λ_1 being $(1^2 + 2^2 + 3^2 + 4^2)/10 = 3.0$ in contrast to the erroneous published value of $(1^2 + 2^2 + 3^2)/10 = 1.4$. The checks provided by (30) are

$$\begin{aligned}
1.1 + 0.0 - 0.3 - 0.8 &= 0 \\
3.6 + 0.0 - 1.2 - 2.4 &= 0 \\
6.3 - 0.3 - 1.2 - 4.8 &= 0 \\
8.0 - 0.3 - 2.4 - 4.8 &= 0 .
\end{aligned}$$

Calculation of the other λ's and f's follows similarly, the results being as shown in Table 2.

(Show Table 2)

The matrix D is as published:

$$D = \begin{bmatrix} .053824 & .036902 & .025373 \\ .036902 & .063205 & .025393 \\ .025373 & .025393 & .056530 \end{bmatrix} .$$

With this and the values shown in Table 2, the value of k_3 obtained from (29) is

$$k_\beta = 59.62 + .053824(539.8726) + .063205(451.3376) + .056530(250.2976)$$
$$-2[.036902(348.7124) + .025373(77.5776) + .025393(45.5376)]$$
$$= 59.62 + 71.7342 - 2(15.9929)$$
$$= 59.62 + 71.73 - 31.98$$
$$= 99.37 \; .$$

The published value was 77.16.

A further numerical error is that for $r' = (-3900 \quad -200 \quad 900)$ the published value of $R_\beta = r'Dr$, using the D given above is 736703, whereas its correct value is

$$3900^2(.053824) + 200^2(.063205) + 900^2(.056530)$$
$$+2(3900)(200)(.036902) - 2(3900)(900)(.025373) - 2(900)(200)(.025393)$$
$$= 737287.72 \; .$$

Summary of corrections

The necessary corrections, noted above, are as follows.

The first is trivial, the second and third relate to typographical errors, the fourth is importand and the last corrects an arithmetical deficiency.

1. At the bottom of page 610 the equations should read

$$R(\mu,\alpha,\beta) = (y' \quad z') \begin{bmatrix} A & B \\ B' & D \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix}$$
$$= (y'Ay + z'B'y + y'Bz + z'Dz)$$
$$= tr(Ayy' + 2Bzy' + z'Dz) \; .$$

(The two B''s are published as B.)

2. In equation (15) the first "2" should be omitted.

3. In the expression for k_β on page 612 the "2" should be omitted from the last term.

4. In the definition of U following equation (15) the elements are $\sum_{j=1}^{b} n_{ij}^2$, with the upper limit of summation being b and not b-1; and V has order b-1 by a with elements $v_{ji} = n_{ij}^2$. Consequences of the correction to U are as follows.

   (a) On page 612, λ_i should be $\sum_{j=1}^{b} n_{ij}^2/n_{i.}$, with upper limit of summation b and not b-1.

   (b) Equation (16) can be replaced by $\sum_{j'=1}^{b} f_{i,jj'} = 0$ for all i and j.

   (c) The computed values of Table 2 on page 615 are as in Table 2 herewith.

   (d) The computed value of k_β on page 615 is 99.37 and not 77.16.

5. The computed value of $R_\beta = \mathbf{r}'D\mathbf{r}$ on page 614 is 737288 and not 736703.

Acknowledgement

Grateful thanks go to W. R. Harvey of Ohio State University for bringing to my notice the errors corrected here.

References

Searle, S. R., and Henderson, C. R. (1960). Judging the effectiveness of age-correction factors. J. Dairy Sci., 43, 966-974.

Searle, S. R., and Henderson, C. R. (1961). Computing procedures for estimating components of variance in the two-way classification, mixed model. Biometrics, 17, 607-616.

Table 1

Hypothetical Example

i	Number of observations n_{ij}					Mean observed values, $x_{i.}$
	j				Totals	
	1	2	3	4	$n_{i.}$	
1	1	2	3	4	10	200
2	3	6	4	7	20	300
3	12	–	12	16	40	400
4	12	12	13	13	50	500
5	25	25	–	–	50	600
Totals $n_{.j}$	53	45	32	40	$n_{..}$ = 170	
Totals of observed values, $x_{.j.}$	23000	23000	14000	19000		

Table 2

Terms used in calculating k_β

i	λ_i	$f_{i,11}$	$f_{i,22}$	$f_{i,33}$	$f_{i,44}$	$-f_{i,12}$	$-f_{i,13}$	$-f_{i,14}$	$-f_{i,23}$	$-f_{i,24}$	$-f_{i,34}$
1	3.0	1.1	3.6	6.3	8.0	0.0	.3	.8	1.2	2.4	4.8
2	5.5	8.775	24.3	14.0	28.175	3.15	.9	4.725	5.4	15.75	7.7
3	13.6	106.56	–	106.56	138.24	–	37.44	69.12	–	–	69.12
4	12.52	110.9376	110.9376	123.4376	123.4376	33.0624	38.9376	38.9376	38.9376	38.9376	45.5624
5	25.0	312.5	312.5	–	–	312.5	–	–	–	–	–
Total	59.62	539.8726	451.3376	250.2976	297.8526	348.7124	77.5776	113.5826	45.5376	57.0876	127.1824

Note: the last 6 columns are prefixed by minus signs.