ON QUADRATIC ESTIMATES OF VARIANCE COMPONENTS[1]

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1. Summary. In this paper quadratic estimates of variance components are considered. For the general balanced nested classification with no specific distributions assumed, it is shown that the quadratic estimate which is unbiased and which has minimum variance is given by the analysis of variance method of estimating the variance components.

2. Introduction. Consider the general balanced nested classification which is described by the model

$$Y_{ijk\cdots p} = \mu + a_i + b_{ij} + c_{ijk} + d_{ijkm} + \cdots + e_{ijk\cdots p}.$$

If all the components are fixed except $e_{ijk\cdots p}$, and if $e_{ijk\cdots p}$ are uncorrelated random variables with means zero, variance σ^2 and with finite fourth moments, then Hsu [1] has shown that the best (minimum variance) quadratic unbiased estimate of σ^2 is given by the analysis of variance method of estimating σ^2.

If we assume a distribution for the $e_{ijk\cdots p}$, then we can get the maximum likelihood estimate for σ^2. However, this method does not tell us how the variance of this estimate compares with the variance of estimates obtained by other methods for finite-sized samples (except for efficient estimates).

If a_i, b_{ij}, c_{ijk}, $\cdots$, $e_{ijk\cdots p}$ are uncorrelated random variables with means zero, variances σ_a^2, σ_b^2, σ_c^2, $\cdots$, and σ^2 respectively, then Crump [2] gives methods for estimating σ_a^2, σ_b^2, σ_c^2, $\cdots$, and σ^2 by making an analysis of variance table, equating expected to observed mean squares and using the solutions to these equations as the estimates. These estimates are quadratic functions of the observations and are unbiased, but very little has been said about the size of the variance of these estimates relative to estimates given by other methods of estimation. Proofs will be given for the two-fold classification only, but they generalize without great difficulty. Theorems will be stated for the general case.

3. Notations and definitions. Consider the linear model

(3.1) $\quad Y_{ijk} = \mu + a_i + b_{ij} + e_{ijk}, \qquad i = 1 \cdots N_1; j = 1 \cdots N_2; k = 1 \cdots N_3,$

where Y_{ijk} is the observation; μ is a constant; and the a_i, b_{ij}, and e_{ijk} are independent chance variables with means zero, variances σ_a^2, σ_b^2, and σ^2, respectively, third moments B_a^3, B_b^3, and B^3, respectively, and finite fourth moments α_a^4, α_b^4, and α^4, respectively. The problem is to estimate σ_b^2 by quadratic functions of the observation Y_{ijk}.

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Definition 1. By the best quadratic unbiased estimate (*BQUE*) of σ_b^2 we will mean a quadratic form Q which satisfies the following:

$$\text{(3.2)} \qquad \text{(a) } EQ = \sigma_b^2, \qquad \text{(b) } \operatorname{var} Q \leqq \operatorname{var} Q^*,$$

where Q^* is any other quadratic form in the observations satisfying (a). (E denotes mathematical expectation, var denotes variance.)

Definition 2. Let a general quadratic form Q be denoted by

$$Q = \sum_{ijk;rst} Y_{ijk} Y_{rst} q_{ijk}^{rst}.$$

The quadratic form given by the analysis of variance method of estimating σ_b^2 is $M = \sum Y_{ijk} Y_{rst} m_{ijk}^{rst}$, where the elements m_{ijk}^{rst} are as follows:

$$\text{(3.3)} \qquad m_{ijk}^{rst} = \begin{cases} \text{(a)} \quad \dfrac{-1}{N_1 N_2 N_3^2 (N_2 - 1)} & r = i;\ s \neq j, \\ \text{(b)} \quad \dfrac{1}{N_1 N_2 N_3 (N_3 - 1)} & r = i;\ s = j;\ t \neq k, \\ \text{(c)} \quad 0 & \text{all other values of } ijkrst. \end{cases}$$

The following relations can be obtained from (3.3):

$$\text{(3.4)} \qquad \begin{array}{ll} \text{(a) } \sum_{ijk} m_{ijk}^{rst} = 0 \text{ for any } r, s, t. & \text{(b) } \sum_{rst} m_{ijk}^{rst} = 0 \text{ for any } i, j, k. \\ \text{(c) } \sum_{jk} m_{ijk}^{rst} = 0 \text{ for any } r, s, t, i. & \text{(d) } \sum_{st} m_{ijk}^{rst} = 0 \text{ for any } i, j, k, r. \end{array}$$

$$\text{(e) } \sum_{ij;tk} m_{ijk}^{ijt} = 1.$$

Theorem I. *In the model given by* (3.1) *the BQUE estimate of* σ_b^2 *is given by the method of analysis of variance, that is, by the quadratic form M stated in* (3.3).

Proof. Let

$$\text{(3.5)} \qquad D = \sum Y_{ijk} Y_{rst} d_{ijk}^{rst} \quad \text{where} \quad q_{ijk}^{rst} = m_{ijk}^{rst} + d_{ijk}^{rst},$$

which implies $Q = M + D$. The problem is to give exact specification to each q_{ijk}^{rst} so that Q satisfies (3.2) or, since m_{ijk}^{rst} are known, the problem reduces to giving exact specification to each d_{ijk}^{rst}. To satisfy (3.2a) we must have $E(Q) = E(M) + E(D) = \sigma_b^2$. This reduces to

$$\text{(3.6)} \qquad \begin{aligned} &\sum_R \mu^2 (d_{ijk}^{rst} + m_{ijk}^{rst}) + \sigma_a^2 \sum_{R(r=i)} (m_{ijk}^{rst} + d_{ijk}^{rst}) \\ &\quad + \sigma_b^2 \sum_{R(r=i, j=s)} (d_{ijk}^{rst} + m_{ijk}^{rst}) + \sigma^2 \sum_{R(r=i; j=s; k=t)} (d_{ijk}^{rst} + m_{ijk}^{rst}) = \sigma_b^2, \end{aligned}$$

where the summation index R refers to summing over all values of the indexes with the restriction in parenthesis. For example, under the second summation sign the symbol $R(r = i)$ means sum over $i = 1 \cdots N_1$; $r = 1 \cdots N_1$; $j = 1 \cdots N_2$; $s = 1 \cdots N_2$; $k = 1 \cdots N_3$; $t = 1 \cdots N_3$; with the restriction $r = i$.

Equating coefficients in (3.6) and using (3.3), we get the following conditions on d_{ijk}^{rst} :

$$(3.7)\qquad \begin{aligned} &(a)\quad \sum_R d_{ijk}^{rst} = 0 &&(b)\quad \sum_{R(r=i)} d_{ijk}^{rst} = 0 \\ &(c)\quad \sum_{R(r=i,j=s)} d_{ijk}^{rst} = 0 &&(d)\quad \sum_{R(r=i;j=s;k=t)} d_{ijk}^{rst} = 0. \end{aligned}$$

Now

$$\text{var } Q = E\,[\sum_R Y_{ijk}Y_{rst}(m_{ijk}^{rst} + d_{ijk}^{rst})]^2 - \sigma_b^4$$

$$(3.8)\qquad = E\,[\sum_R Y_{ijk}Y_{rst}\,m_{ijk}^{rst}]^2 + E\,[\sum_R Y_{ijk}Y_{rst}\,d_{ijk}^{rst}]^2$$

$$+ 2E\,[\sum_R Y_{ijk}Y_{rst}m_{ijk}^{rst}\sum_P Y_{fgh}Y_{uvw}\,d_{fgh}^{uvw}] - \sigma_b^4$$

where the index P is defined for the subscripts f, g, h, u, v, w, the same as R was defined for i, j, k, r, s, t. We will examine the last term of (3.8) in detail. Let us first examine the quantity

$$(3.9)\qquad \sum_R Y_{ijk}Y_{rst}m_{ijk}^{rst}.$$

Substituting (3.1) into (3.9) we get

$$\sum_R (\mu + a_i + b_{ij} + e_{ijk})(\mu + a_r + b_{rs} + e_{rst})m_{ijk}^{rst},$$

which in virtue of (3.4c) and (3.4d) reduces to

$$\sum_R (b_{ij} + e_{ijk})(b_{rs} + e_{rst})m_{ijk}^{rst}.$$

Thus the third term of (3.8), omitting the coefficient 2, reduces to

$$(3.10)\qquad E\,[\sum_R\sum_P (b_{ij} + e_{ijk})(b_{rs} + e_{rst})(\mu + a_f + b_{fg} + e_{fgh})$$

$$(\mu + a_u + b_{uv} + e_{uvw})m_{ijk}^{rst}d_{fgh}^{uvw}].$$

Due to (3.7a), this term, which we may denote by C, will contain no terms involving μ^2. Due to (3.7b), C will contain no terms involving σ_a^2, since this would force $u = f$ in d_{fgh}^{uvw} and $\sum_{P(u=f)} d_{fgh}^{uvw} = 0$ by (3.7b). Since each of the a_i, b_{ij}, and e_{ijk} are independent with means zero, the expectation of any term in C involving these elements linearly will be zero. Neither can C contain a term which involves μ linearly, since this would be one of the forms μB^3 or μB_b^3. But terms such as μB^3 could come only from elements of e_{ijk} and e_{rst} when $i = r$; $j = s$; and $k = t$. When these corresponding subscripts are equal the term vanishes by (3.3c).

Also terms such as μB_b^3 could come only from elements such as $\mu b_{ij}b_{rs}b_{fg}$ with $i = r = f$ and $j = s = g$, or $\mu b_{ij}b_{rs}b_{uv}$ with $i = r = u$ and $j = s = v$. Thus we would get (from $\mu b_{ij}b_{rs}b_{fg}$)

$$\mu B_b^3 \sum_{ijkt}\sum_{uvwh} m_{ijk}^{ijt}d_{ijh}^{uvw} = \mu B_b^3 \sum_{uvw;ihj} d_{ijh}^{uvw}\sum_{kt} m_{ijk}^{ijt} = \mu B_b^3 \sum_{uvw;ijh} d_{ijh}^{uvw}\frac{1}{N_1N_2}$$

$$= \frac{1}{N_1N_2}\mu B_b^3 \sum_{ijh;uvw} d_{ijh}^{uvw}.$$

This is zero by (3.7a). Now let us examine terms of C which lead to terms involving $\sigma_b^2\sigma^2$. This can come from only six terms:

$$(1) \qquad E\sum_R\sum_P b_{ij}b_{rs}e_{fgh}e_{uvw}m_{ijk}^{rst}d_{fgh}^{uvw} = \sigma_b^2\sigma^2\sum_{ijkt;uvw} m_{ijk}^{ijt}d_{uvw}^{uvw}.$$

This is zero by (3.7d).

$$(2) \qquad E\sum_R\sum_P b_{fg}b_{uv}e_{ijk}e_{rst}m_{ijk}^{rst}d_{fgh}^{uvw} = \sigma_b^2\sigma^2\sum_{ijk;uvwh} m_{ijk}^{ijk}d_{uvh}^{uvw}.$$

This is zero by (3.3c).

$$(3) \qquad E\sum_R\sum_P b_{ij}b_{uv}e_{rst}e_{fgh}m_{ijk}^{rst}d_{fgh}^{uvw} = \sigma_b^2\sigma^2\sum_{ijkw;rst} m_{ijk}^{rst}d_{rst}^{ijw}.$$

This is zero by (3.3) unless $r = i$. If $r = i$, we get

$$\sum_{ijkw;rst} m_{ijk}^{rst}d_{rst}^{ijw} = \sum_{ijkwt;s\neq j} m_{ijk}^{ist}d_{ist}^{ijw} + \sum_{ijkwt} m_{ijk}^{ijt}d_{ijt}^{ijw}$$
$$= \sum_{ijwt;s\neq j} d_{ist}^{ijw}\sum_k m_{ijk}^{ist} + \sum_{ijwtk} d_{ijt}^{ijw}m_{ijk}^{ijt}.$$

Using (3.3) this becomes

$$\sum_{ijwt;s\neq j} d_{ist}^{ijw}\left(\frac{-1}{N_1N_2N_3(N_2-1)}\right) + \sum_{ijwt} d_{ijt}^{ijw}\left(\frac{1}{N_1N_2N_3}\right).$$

This is zero by (3.7b) and (3.7c). The remaining three terms are:

$$(4) \qquad E\sum_R\sum_P b_{rs}b_{fg}e_{ijk}e_{uvw}m_{ijk}^{rst}d_{fgh}^{uvw} = \sigma_b^2\sigma^2\sum_{rstijkh} m_{ijk}^{rst}d_{rsh}^{ijk}$$

$$(5) \qquad E\sum_R\sum_P b_{ij}b_{fg}e_{rst}e_{uvw}m_{ijk}^{rst}d_{fgh}^{uvw} = \sigma_b^2\sigma^2\sum_{ijkh;rst} m_{ijk}^{rst}d_{ijh}^{rst};$$

$$(6) \qquad E\sum_R\sum_P b_{rs}b_{uv}e_{ijk}e_{fgh}m_{ijk}^{rst}d_{fgh}^{uvw} = \sigma_b^2\sigma^2\sum_{ijkw;rst} m_{ijk}^{rst}d_{ijk}^{rsw}.$$

Each of these three, (4), (5), and (6), is zero by the same argument as used for part (3). Thus we have reduced C to two terms, (A) and (B):

$$(A) = E\sum_R\sum_P b_{ij}b_{rs}b_{fg}b_{uv}m_{ijk}^{rst}d_{fgh}^{uvw}$$
$$(B) = E\sum_R\sum_P e_{ijk}e_{rst}e_{fgh}e_{uvw}m_{ijk}^{rst}d_{fgh}^{uvw}.$$

Let us examine these in detail. We see that (A) is zero unless the subscripts fit one of the following four models:

$A.1$ $i = r; j = s; f = u; g = v$ where either $i \neq f$ or $j \neq g$.
$A.2$ $i = f; j = g; r = u; s = v$ where either $i \neq r$ or $j \neq s$.
$A.3$ $i = u; j = v; r = f; s = g$ where either $i \neq r$ or $j \neq s$.
$A.4$ $i = r = f = u; j = s = g = v$.

For case $A.1$, (A) reduces to zero by (3.7c). In case $A.2$, if $i \neq r$, then $(A) = 0$ by (3.3c). If $i = r$, we get

$$(A) = \sigma_b^4\sum_{ijst;khw;s\neq j} m_{ijk}^{ist}d_{ijh}^{isw} = \sigma_b^4\sum_{ijst;khw;s\neq j}\left(\frac{-1}{N_1N_2N_3^2(N_3-1)}d_{ijh}^{isw}\right),$$

which is zero by (3.7b) and (3.7c). For case $A.3$, (A) is zero by an argument identical with that for case $A.2$. For case $A.4$, we get

$$(A) = \alpha_b^4 \sum_{ijkthw} m_{ijk}^{ijt} d_{ijh}^{ijw}$$

which is zero by (3.7c). Thus (A) is equal to zero.

Now for (B). We immediately see that (B) is zero unless the subscripts fit one of the following four cases.

$B.1$ $i = r; j = s; k = t; f = u; g = v; h = w$ where $i \neq f; j \neq g$; or $k \neq h$.

$B.2$ $i = f; j = g; k = h; r = u; s = v; t = w$ where either $i \neq r; j \neq s$; or $k \neq t$.

$B.3$ $i = u; j = v; k = w; r = f; s = g; t = h$ where either $i \neq r; j \neq s$; or $k \neq t$.

$B.4$ $i = r = f = u; j = s = g = v; k = t = h = w$.

For case $B.1$ we get

$$(B) = \sigma^4 \sum_{ijk;fgh} m_{ijk}^{ijk} d_{fgh}^{fgh} \qquad \text{with either } i \neq f; j \neq g \text{ or } k \neq h;$$

but this is zero by (3.7d). For case $B.2$ we get

$$(B) = \sigma^4 \sum_{ijk;rst} m_{ijk}^{rst} d_{ijk}^{rst} \qquad \text{with either } i \neq r; j \neq s; \text{ or } k \neq t.$$

If $i \neq r$, this is zero by (3.3c). If $i = r$, we get

$$(B) = \sigma^4 \sum_{ijk;st} m_{ijk}^{ist} d_{ijk}^{ist} \qquad \text{with either } j \neq s \text{ or } k \neq t.$$

If $j \neq s$, we get, using (3.3a),

$$(B) = \sigma^4 \sum_{ijkt;s\neq j} \left(\frac{-1}{N_1 N_2 N_3^2 (N_2 - 1)}\right) d_{ijk}^{ist}$$

which is zero by (3.7b) and (3.7c). If $j = s$ and $k \neq t$, we get

$$(B) = \sigma^4 \sum_{ijkt;k\neq t} \left(\frac{1}{N_1 N_2 N_3 (N_3 - 1)}\right) d_{ijk}^{ijt}$$

which is zero by (3.7c) and (3.7d). Thus (B) is equal to zero for case $B.2$. For case $B.3$ (B) is zero by an argument identical with the argument for $B.2$. For case $B.4$ we get

$$(B) = \alpha^4 \sum_{ijk} m_{ijk}^{ijk} d_{ijk}^{ijk}.$$

But this is zero by (3.3c). Thus (B) is equal to zero.

We have thus proved that C is zero, and (3.8) becomes

$$\operatorname{var} Q = E \left[\sum_R Y_{ijk} Y_{rst} m_{ijk}^{rst}\right]^2 + E \left[\sum_R Y_{ijk} Y_{rst} d_{ijk}^{rst}\right]^2,$$

but this is a minimum if $d_{ijk}^{rst} = 0$. These values are also consistent with the conditions of unbiasedness. This proves the theorem. By methods similar to above, it can be shown that the $BQUE$ estimate of σ_a^2 (or of σ^2) is given by the analysis of variance method of estimating variance components.

4. The k-fold classification. Let the random variable $Y_{i_1 i_2 \cdots i_k}$ be given by

$$Y_{i_1 i_2 \cdots i_k} = \mu + a_{i_1}^{(1)} + a_{i_1 i_2}^{(2)} + a_{i_1 i_2 i_3}^{(3)} + \cdots + a_{i_1 i_2 \cdots i_k}^{(k)} \tag{4}$$

where $i_j = 1 \cdots n_j$ and μ is a constant and the $a^{(t)}$ are independent random variables with the following properties:

$$E(a_{i_1 i_2 \cdots i_t}^{(t)}) = 0 \qquad \text{var } a_{i_1 i_2 \cdots i_t}^{(t)} = \sigma_t^2 \qquad E(a_{i_1 i_2 \cdots i_t}^{(t)})^4 = \mu_{4t} < \infty \qquad t = 1 \cdots k.$$

This is the general balanced nested (hierarchal) classification.

THEOREM II. *The best quadratic unbiased estimate of σ_t^2 (denoted by $\hat{\sigma}_t^2$) in the model defined by* (4) *is given by the analysis of variance.*

THEOREM III. *The variance of $\hat{\sigma}_t^2$ is given by*

$$\frac{2(n_t n_{t+1} - 1)}{N_1 N_{t+1}(n_t - 1)(n_{t+1} - 1)} \left[2 \sum_{p=t+1}^{k-1} \sum_{q=p+1}^{k} N_{p+1} N_{q+1} \sigma_p^2 \sigma_q^2 + \sum_{p=t+1}^{k} N_{p+1}^2 \sigma_p^4 \right]$$
$$+ \frac{4 n_t \sigma_t^2}{N_1(n_t - 1)} \sum_{q=t+1}^{k} N_{q+1} \sigma_q^2 + \frac{N_{t+1}}{N_1} (\mu_{4t} - 3\sigma_t^4) + \frac{2N_t}{N_1(n_t - 1)} \sigma_t^4,$$

where $N_u = n_u n_{u+1} \cdots n_k$ if $u \leqq k$ and $N_u = 1$ if $u > k$.

THEOREM IV. *Under the model defined in* (4), *the best quadratic unbiased estimate of $\sum_{i=1}^k g_i \sigma_i^2$ (where g_i are known constants) is given by $\sum_{i=1}^k g_i \hat{\sigma}_i^2$.*

This is proven by a method similar to the method used to prove Theorem I.

THEOREM V. *The variance of $[\sum_{i=1}^k g_i \hat{\sigma}_i^2]$ is*

$$\sum_{i=1}^{k} g_i^2 \text{ var } \hat{\sigma}_i^2 - \frac{4}{N_1} \sum_{i=1}^{k-1} \frac{g_i g_{i+1}}{N_{i+2}(N_{i+1} - 1)} \left[\sum_{p=i+1}^{k} N_{p+1} \sigma_p^2 \right]^2.$$

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