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Estimators of Repeatability*

H. Mansour, E.V. Nordheim and J.J. Rutledge
University of Wisconsin, Madison, Wis. (USA)

Summary. Analysis of variance and principal components methods have been suggested for estimating repeatability. In this study, six estimation procedures are compared: ANOVA, principal components based on the sample covariance matrix and also on the sample correlation matrix, a related multivariate method (structural analysis) based on the sample covariance matrix and also on the sample correlation matrix, and maximum likelihood estimation. A simulation study indicates that when the standard linear model assumptions are met, the estimators are quite similar except when the repeatability is small. Overall, maximum likelihood appears the preferred method. If the assumption of equal variance is relaxed, the methods based on the sample correlation matrix perform better although others are surprisingly robust. The structural analysis method (with sample correlation matrix) appears to be best.

Key words: Estimation – Repeatability – Linear models Multivariate analysis

Introduction

Repeatability is a measure of 'the extent to which differences between individuals depend on genetic and permanent environmental effects, rather than on those which are temporary' (Turner and Young 1969). Analysis of variance methods have traditionally been used to estimate repeatability. More recently, multivariate methods using principal components have been suggested (Abeywardena 1972; Rutledge 1974). Our first objective is to compare the ANOVA and principle components methods along with some others. This will include a brief discussion of properties and some simulations.

In traditional estimation of repeatability, the standard linear model assumption of independent errors having common variance is made. As a second objective, we briefly explore the performance of the various estimation procedures for the case when the assumption of variance homogeneity is relaxed. Application to an example of mouse litter size data will be made.

Estimators of Repeatability

A standard linear model often used to describe the production or yield of an animal or plant is:

$$Y_{ij} = \mu + a_i + \tau_j + e_{ij} \quad i = 1 \dots n; \quad j = 1 \dots k \qquad (1)$$

where Y_{ij} is the production or yield, μ is an overall (fixed) mean, a_i is a random effect for individual, τ_j is a fixed time effect and e_{ij} is a random error. The usual assumptions made are:

$$a_i \sim N(0, \sigma_a^2); \quad e_{ij} \sim N(0, \sigma_e^2); \quad \sum_{j=1}^{k} \tau_j = 0$$

with all a_i and e_{ij} terms independent. We shall consider only cases where each individual has a record in each time period (balanced data). In some applications the τ_j term is suppressed from (1), but we shall not further consider this case. A standard analysis of this balanced mixed model leads to the ANOVA table: (see following page)

By equating the mean square of each source to its expectation, estimates of σ_e^2 and σ_a^2 can be obtained. The estimators are:

$$\hat{\sigma}_e^2 = \text{MSE}, \quad \hat{\sigma}_a^2 = (\text{MSA} - \text{MSE})/k$$

where MSA and MSE are the mean squares for individual and error respectively. The corresponding estimator of repeatability (ρ) is:

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Source	Degrees of freedom	Mean square	Expected mean square
Individual	n − 1	$k \sum_{i=1}^{n} (\bar{Y}_{i.} - \bar{Y}_{..})^2/(n-1)$	$\sigma_e^2 + k\sigma_a^2$
Time	k − 1	$n \sum_{j=1}^{k} (\bar{Y}_{.j} - \bar{Y}_{..})^2/(k-1)$	$\sigma_e^2 + \frac{n}{k-1} \sum_{j=1}^{k} \tau_j^2$
Error	(n − 1)(k − 1)	$\sum_{i=1}^{n} \sum_{j=1}^{k} (Y_{ij} - \bar{Y}_{i.} - \bar{Y}_{.j} + \bar{Y}_{..})^2/(n-1)(k-1)$	σ_e^2

$$\hat{\rho}_{AO} = \hat{\sigma}_a^2/(\hat{\sigma}_a^2 + \hat{\sigma}_e^2) = (MSA - MSE)/[MSA + (k-1)MSE] \quad (2)$$

(The ANOVA estimator obtained when the τ_j term is deleted from (1) is the intraclass correlation).

Model (1) can be formulated multivariately:

$$\underset{\sim}{Y}_i = (Y_{i1}, Y_{i2}, ..., Y_{ik})' \sim N_k \left[\begin{bmatrix} \mu_1 \\ \mu_2 \\ \cdot \\ \cdot \\ \mu_k \end{bmatrix}, \sigma_t^2 \begin{bmatrix} 1 & \rho & \ldots & \rho \\ \rho & 1 & \ldots & \rho \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \rho & \rho & \ldots & 1 \end{bmatrix} \right] \quad (3)$$

where $\mu_j = \mu + \tau_j$, $\sigma_t^2 = \sigma_a^2 + \sigma_e^2$ and $\rho = \sigma_a^2/(\sigma_a^2 + \sigma_e^2)$. The correlation ρ is the repeatability and σ_t^2 is the phenotypic variance.

The component structure of the covariance matrix in (3) is discussed in Morrison (1976). The largest characteristic root is:

$$\lambda_v = \sigma_t^2 [1 + (k-1)\rho] \quad (4)$$

with corresponding vector $\underset{\sim}{b}$

$$\underset{\sim}{b}' = (1/\sqrt{k}, ..., 1/\sqrt{k}). \quad (5)$$

From (4) it follows that an estimator for ρ is:

$$\hat{\rho}_{PV} = [\hat{\lambda}_v/\hat{\sigma}_t^2 - 1]/[k-1] \quad (6)$$

where $\hat{\lambda}_v$ is the largest characteristic root from the sample covariance matrix, S, and $\hat{\sigma}_t^2$ is an estimator of the phenotypic variance. Herein S denotes the usual unbiased sample covariance matrix. From (3), a natural estimator of σ_t^2 is the mean of the diagonal terms from S.

If principal components are extracted from the correlation matrix corresponding to (3), the largest characteristic root is the same as in (4) with σ_t^2 replaced by 1 and the characteristic vector is as in (5). A reasonable estimator (Rutledge 1974) in this case is:

$$\hat{\rho}_{PR} = [\hat{\lambda}_r - 1]/[k-1] \quad (7)$$

where $\hat{\lambda}_r$ is the largest characteristic root from the sample correlation matrix, R.

A multivariate procedure related to principal components recalls the basic definition of principal components. With V as the 'theoretical' covariance matrix, the first principal component is the vector $\underset{\sim}{a}$ that maximizes $\underset{\sim}{a}'V\underset{\sim}{a}$ subject to the constraint that $\underset{\sim}{a}'\underset{\sim}{a} = 1$. It follows that $\lambda_v = \max \underset{\sim}{a}'V\underset{\sim}{a}$. Since the structure in (3) leads to first principal component $\underset{\sim}{b}$ from (5), another possible estimator of ρ is:

$$\hat{\rho}_{SV} = [\underset{\sim}{b}'S\underset{\sim}{b}/\hat{\sigma}_t^2 - 1]/[k-1] \quad (8)$$

This procedure can also be applied to the correlation matrix. The resulting estimator is:

$$\hat{\rho}_{SR} = [\underset{\sim}{b}'R\underset{\sim}{b} - 1]/[k-1] \quad (9)$$

To distinguish the estimators (8) and (9), they will be referred to as having come from a structural analysis.

A final estimator we consider here is the maximum likelihood estimator with σ_a^2 constrained to be non-negative. Following Searle (1971), this estimator is:

$$\hat{\rho}_{ML} = \max \{(MSA - MSE)/[MSA + (k-1)MSE], 0\} = \max \{\hat{\rho}_{AO}, 0\} \quad (10)$$

We note that the close relationship between $\hat{\rho}_{ML}$ and $\hat{\rho}_{AO}$ does not hold exactly if the τ_i term is deleted from (1). (See Appendix for brief discussion).

A tabulation of estimators for easy reference is given as Table 1.

Table 1. List of estimators

$\hat{\rho}_{AO}$	ANOVA estimator
$\hat{\rho}_{PV}$	Estimator based on principal components extracted from sample covariance matrix
$\hat{\rho}_{PR}$	Estimator based on principal components extracted from sample correlation matrix
$\hat{\rho}_{SV}$	Structural estimator from sample covariance matrix using (theoretical) vector corresponding to largest characteristic root (this estimator is identical to $\hat{\rho}_{AO}$)
$\hat{\rho}_{SR}$	Structural estimator from sample correlation matrix using (theoretical) characteristic vector corresponding to largest characteristic root
$\hat{\rho}_{ML}$	Maximum likelihood estimator with $\sigma_a{}^2$ constrained to be non-negative

Interpretation and Comparison of Estimators

The ANOVA estimator, $\hat{\rho}_{AO}$ can take on negative values. This occurs if and only if $\hat{\sigma}_a^2$ is negative. In a sense the MLE $\hat{\rho}_{ML}$ can be viewed as the ANOVA estimator that replaces $\hat{\sigma}_a^2$ by 0 if $\hat{\sigma}_a^2$ is negative. The structural estimators $\hat{\rho}_{SV}$ and $\hat{\rho}_{SR}$ can also be negative, whereas the principal components estimators $\hat{\rho}_{PV}$ and $\hat{\rho}_{PR}$ are constrained to be positive since $\hat{\lambda}_v \geq \hat{\sigma}_t^2$ and $\hat{\lambda}_r \geq 1$, by definition. The drawback to the non-negativity of $\hat{\rho}_{PV}$, $\hat{\rho}_{PR}$ and $\hat{\rho}_{ML}$ is the occurrence of a non-negligible bias when (true) ρ is small. We note that $\hat{\rho}_{AO}$ and $\hat{\rho}_{SR}$ have small though negligible bias.

Formal statistical properties of the estimators are difficult to derive. Some progress is possible when k = 2, but this will not be pursued here. An estimate of the asymptotic standard error (ASE) for $\hat{\rho}_{AO}$ is well known and is given, for example, in Turner and Young (1969).

$$\sigma_{\hat{\rho}_{AO}} = (1-\hat{\rho})\,[1 + (k-1)\hat{\rho}]/[1/2\,k\,(k-1)\,(n-1)]^{1/2}. \tag{11}$$

Anderson (1951) has demonstrated a result from which it follows that $\sigma_{\hat{\rho}_{PR}}$ has ASE given by (11) when $\rho > 0$.

It can be shown by straightforward algebra that $\hat{\rho}_{AO}$ is equal to the average covariance divided by the average variance from S (Winer 1971). It is also easy to show that $\hat{\rho}_{SV}$ is equal to the same quantity. Thus,

$$\hat{\rho}_{AO} = \hat{\rho}_{SV} = \left[\frac{1}{k(k-1)} \sum_{j=1}^{k} \sum_{\substack{j'=1 \\ j \neq j'}}^{k} s_{jj'}\right] \Bigg/ \left[\frac{1}{k} \sum_{j=1}^{k} s_{jj}\right] \tag{12}$$

where $s_{jj'}$ is the element in the j^{th} row and j'^{th} column of S. Similarly, $\hat{\rho}_{SR}$ is equal to the average pairwise correlation

$$\hat{\rho}_{SR} = \frac{1}{k(k-1)} \sum_{j=1}^{k} \sum_{\substack{j'=1 \\ j \neq j'}}^{k} r_{jj'} \tag{13}$$

where $r_{jj'}$ is the element in the j^{th} row and j'^{th} column of R. (We demonstrate this result in the Appendix). Thus, $\hat{\rho}_{AO}$ ($\hat{\rho}_{SV}$) and $\hat{\rho}_{SR}$ have pleasing interpretations. The estimator $\hat{\rho}_{ML}$ relates to $\hat{\rho}_{AO}$ as mentioned earlier. The principal components estimators have no obvious interpretations.

In order to compare our five distinct estimators, we conducted a simulation study. Using a multivariate normal generator, we generated observations according to (3). We considered 5 values for ρ: 0.00, 0.10, 0.25, 0.50, 0.75; 3 values for k (number of records): 2, 4, 6; and 2 values for n (number of individuals): 50, 200. These values were selected primarily to reflect situations of possible interest to animal scientists. For each combination of ρ, k and n, we conducted 100 simulation runs, computing the repeatability for each run using each estimator.

Our basic results are presented in Figs. 1 and 2. Here we display the Monte-Carlo biases and variances for $\rho = 0$ and 0.5 for all values of k and n considered. Monte-Carlo bias is defined as the difference between the computed mean of 100 estimates and ρ. To interpret the results, recall the discussion at the beginning of this section on the algebraic

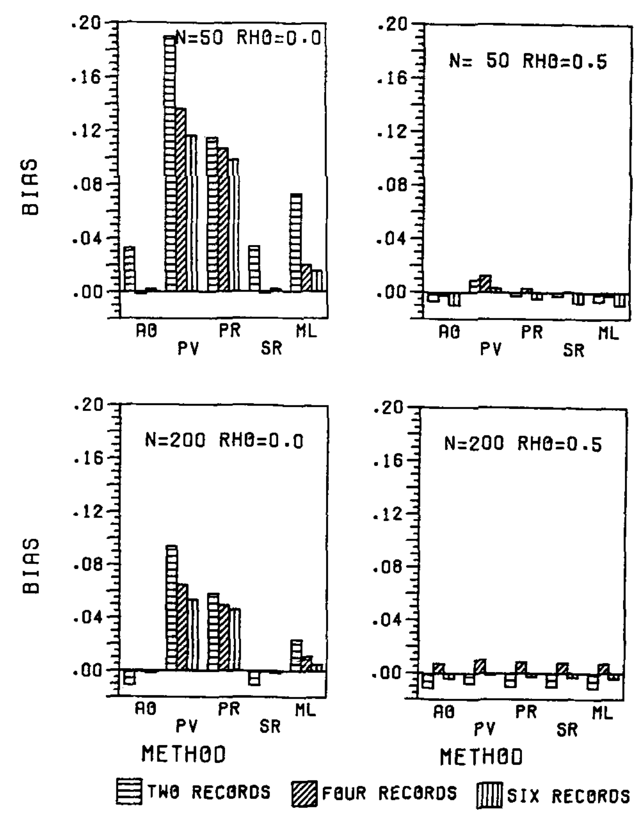

Fig. 1. Monte-Carlo biases (homogeneous variance). Rho (ρ) is the true value of repeatability, and N is the number of individuals

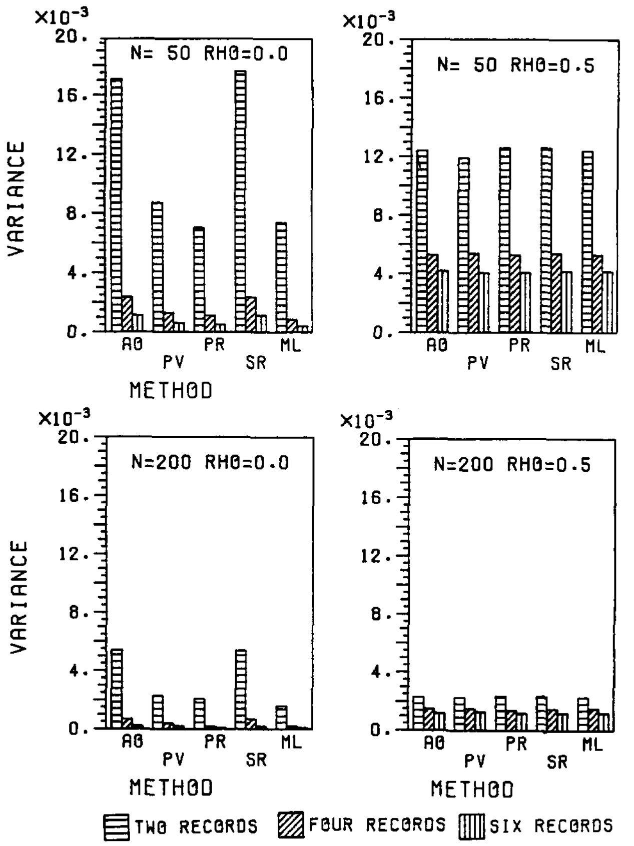

Fig. 2. Monte-Carlo variances (homogeneous variance). Rho (ρ) is the true value of repeatability, and N is the number of individuals

sign of the estimators. Thus, one expects differing behavior of the estimators when ρ is small. The figures confirm this evaluation and also demonstrate performance similarities for larger ρ. The plotted results for $\rho = 0.5$ are typical of the large ρ situation, e.g., comparable Monte-Carlo biases and variances. For $\rho = 0$, we note firstly that $\hat{\rho}_{AO}(\hat{\rho}_{SV})$ and $\hat{\rho}_{SR}$ have negligible bias, $\hat{\rho}_{ML}$ has modest bias, and $\hat{\rho}_{PV}$ and $\hat{\rho}_{PR}$ have larger biases. Secondly, the variances for $\hat{\rho}_{AO}(\hat{\rho}_{SV})$ and $\hat{\rho}_{SR}$ are the largest with the variances for $\hat{\rho}_{PV}$, $\hat{\rho}_{PR}$ and $\hat{\rho}_{ML}$ roughly comparable. (We note that the variances for $\hat{\rho}_{AO}$ with $\rho = 0$ and $\rho = 0.5$ and the variances for all other estimators, including $\hat{\rho}_{PR}$, with $\rho = 0.5$ show close agreement with (11).)

A common method to evaluate estimators is that of mean squared error (MQE) (Bickel and Doksum 1977). This measure is given by the sum of bias squared and variance. For $\rho = 0.5$ the MQE computed from the Monte-Carlo values is similar for all estimators; however, at $\rho = 0$, $\hat{\rho}_{ML}$ has consistently the lowest MQE with the others following the general (increasing) order $\hat{\rho}_{AO}(\hat{\rho}_{SV})$ and $\hat{\rho}_{SR}$, $\hat{\rho}_{PR}$ and $\hat{\rho}_{PV}$. For $\rho = 0.10$, (results not shown) $\hat{\rho}_{PR}$ and $\hat{\rho}_{ML}$ have comparable MQE with the other estimators having slightly higher values.

In general, except for very small ρ, there is rather little difference among estimators. Perhaps $\hat{\rho}_{PV}$ is the least desirable since its behavior is the least consistent. Considering the small ρ case, we conclude that $\hat{\rho}_{ML}$ seems to perform the best, and we would recommend its use.

Robustness When Variances are Unequal

In certain circumstances the assumption of homogeneous variances may not be appropriate; yet the notion of repeatability seems reasonable. In this case the model can be expressed as (3) with covariance matrix replaced by:

$$\Sigma = \begin{bmatrix} \sigma_{11}^2 & \rho\sigma_{11}\sigma_{22} & \dots & \rho\sigma_{11}\sigma_{kk} \\ & \sigma_{22}^2 & \dots & \rho\sigma_{22}\sigma_{kk} \\ & & \dots & . \\ & & & \sigma_{kk}^2 \end{bmatrix} \tag{14}$$

where σ_{jj}^2 is the phenotypic variance of the j^{th} record and ρ is the repeatability. For situations in which the σ_{jj}^2 are unequal, we would expect the estimators based on the sample correlation matrix, $\hat{\rho}_{PR}$ and $\hat{\rho}_{SR}$, to perform better than the others.

A simulation study was carried out with $k = 4$, $n = 200$, $\rho = 0, 0.1, 0.25, 0.5$ and 0.75 and two sets of variances as shown below.

σ_{11}^2	σ_{22}^2	σ_{33}^2	σ_{44}^2
6	7	8	9
6	9	12	15

The results using the second set of variances are shown in Figs. 3 and 4 for estimators $\hat{\rho}_{AO}(\hat{\rho}_{SV})$, $\hat{\rho}_{PR}$, $\hat{\rho}_{SR}$ and $\hat{\rho}_{ML}$. For small correlations we note the same behavior as in the standard case. However, for larger correlations, the estimators not based directly on the sample correlation matrix show a negative Monte-Carlo bias. What appears surprising is the relatively small magnitude of this bias. By calculating the ratio of average (true) covariance to average (true) variance for (14) with $k = 4$ and the second set of variances, we note $\rho_{AO} = 0.964\,\rho$ (this is demonstrated in the Appendix). Thus, $\hat{\rho}_{AO}(\hat{\rho}_{SV})$ and $\hat{\rho}_{ML}$ appear to be quite robust to variance heterogeneity. Taking into account the difficulties with $\hat{\rho}_{PR}$ for small ρ, we feel that $\hat{\rho}_{SR}$ would be a recommended estimator.

As an example of data having such structure, we obtained the litter sizes of 150 randomly-mated ICR mice over their first four parities. (As the litter sizes are typically

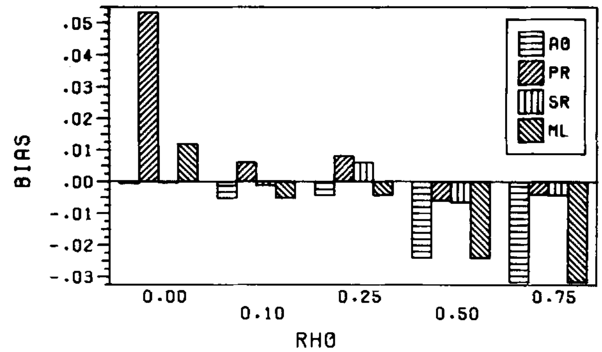

Fig. 3. Monte-Carlo biases (4 records, unequal variances: 6, 9, 12 and 15). Rho (ρ) is the true value of repeatability, N = 200

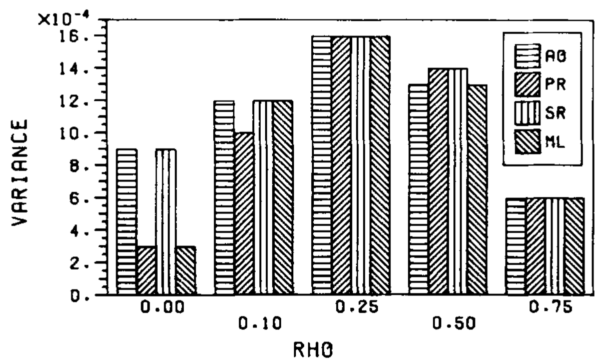

Fig. 4. Monte-Carlo variances (4 records, unequal variances: 6, 9, 12 and 15). Rho (ρ) is the true value of repeatability, N = 200

around 10, we ignore any difficulties due to discrete effects). As shown below, the sample covariance matrix calculated from these data indicates that an assumption of constant variances does not appear plausible, whereas the sample correlation matrix shows that there is a fairly consistent repeatability:

$$S = \begin{bmatrix} 3.50 & 1.40 & 1.14 & 1.27 \\ & 5.22 & 1.38 & 1.73 \\ & & 7.45 & 1.71 \\ & & & 8.50 \end{bmatrix},$$

$$R = \begin{bmatrix} 1 & 0.33 & 0.22 & 0.23 \\ & 1 & 0.22 & 0.26 \\ & & 1 & 0.22 \\ & & & 1 \end{bmatrix}$$

For this case, $\hat{\rho}_{AO}(\hat{\rho}_{SV}) = \hat{\rho}_{ML} = 0.233$, $\hat{\rho}_{PV} = 0.248$ and $\hat{\rho}_{SR} = 0.247$.

Discussion

In the previous sections we considered several estimators of repeatability and compared their performance in a variety of situations including some in which the assumption of homogeneous variances was violated. In general, we found that the estimators behaved similarly although there is, perhaps, a slight preference for $\hat{\rho}_{ML}$ when the variances are close to homogeneous and for $\hat{\rho}_{SR}$ when the variances are inhomogeneous.

Some additional issues warrant mentioning. Firstly, one wishes to know how well these estimators perform when other standard assumptions are violated and if there may be other and better estimators in these cases. This point can only be answered with further work. Secondly, it is important to determine from the data which of the assumptions may be violated. For instance, Wilks (1946) has generalized a likelihood ratio statistic to test for the null hypothesis that the covariance structure is that in (3). However, this procedure appears quite nonrobust to departures from normality and consequently may be of limited usefulness. Thirdly, analysis of unbalanced data is difficult in practice. Although maximum liklihood estimation is in principle straightforward, though tedious, there is no completely satisfactory ANOVA procedure. For methods involving sample covariance and correlation matrices, we observe that there is no universally accepted way to define these matrices. Further developments in multivariate analysis and variance components estimation will be necessary in order to develop a satisfactory methodology. We intend to report on our future progress.

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Appendix

1 Relationship Between $\hat{\rho}_{ML}$ and $\hat{\rho}_{AO}$ when τ_j Term is Deleted from (1)

From Searle (1971), the form of the ANOVA estimator obtained when the τ_j term is deleted from (1) is identical to (2). However, the MLE is max $\{[(n-1)MSA/n - MSE]/[(n-1)MSA/n + (k-1)MSE], 0\}$. For small n the close relationship between estimators noted below (10) does not hold; however, as $(n-1)/n$ approaches 1, the close relationship is approximately valid.

2 Demonstration of Eq. (13)

From (9) $\hat{\rho}_{SR} = [1/k \sum_{j=1}^{k} \sum_{j'=1}^{k} r_{jj'} - 1]/[k-1]$

$$= [1/k(\sum_{j=1}^{k} r_{jj} + \sum_{\substack{j=1 \\ j \neq j'}}^{k} \sum_{j'=1}^{k} r_{jj'}) - 1]/[k-1]$$

$$= \frac{1}{k(k-1)} \sum_{\substack{j=1 \\ j \neq j'}}^{k} \sum_{j'=1}^{k} r_{jj'}.$$

3 Demonstration that $\rho_{AO} = 0.964\ \rho$ from (14) when $\sigma_{11}^2 = 6$, $\sigma_{22}^2 = 9$, $\sigma_{33}^2 = 12$ and $\sigma_{44}^2 = 15$

From (14) with k = 4, $\rho_{AO} (= \rho_{SV}) =$

$$\frac{1}{6} \sum_{\substack{i=1 \\ i<j}}^{4} \sum_{j=2}^{4} \rho\sigma_{ii}\sigma_{jj} / \frac{1}{4} \sum_{i=1}^{4} \sigma_{ii}^2.$$

For the particular values of σ_{ii}, $\rho_{AO} = 0.964\ \rho$.

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Mr. H. Mansour
Dr. J.J. Rutledge
Department of Meat and Animal Science
Room 256, Animal Sciences Building
1675 Observatory Drive
Madison, Wis. 53706 (USA)

Dr. E.V. Nordheim
Department of Statistics and Forestry
University of Wisconsin
Madison, Wis. 53706 (USA)