ON ESTIMATING COVARIANCE COMPONENTS

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Abstract

A well-known formula for expressing a covariance in terms of variances is shown to hold true for estimating components of covariance.

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Covariance components are defined by Rao [1971] as the off-diagonal elements of a variance-covariance matrix that is not diagonal. The more usual way of looking at covariance components, that familiar to geneticists for example, is of having 2 random variables X_1 and X_2, observed in pairs, with components of covariance being the components of the covariance between X_1 and X_2 defined in the same way as are the components of variance of X_1 and of X_2. A simple illustration is the 1-way classification. If x_{1ij} and x_{2ij} are measurements on the j'th unit of the i'th class, the customary random effects models are

$$x_{1ij} = \mu_1 + \alpha_i + e_{ij} \quad \text{and} \quad x_{2ij} = \mu_2 + \beta_i + \epsilon_{ij} \tag{1}$$

where μ_1 and μ_2 are overall means, α_i and β_i are the random effects due to the i'th class and e_{ij} and ϵ_{ij} are the error terms, the variance components being σ^2_α, σ^2_β and σ^2_e, σ^2_ϵ respectively. The covariance components are then $\sigma_{\alpha\beta} = \text{cov}(\alpha_i\beta_i)$ for all i and $\sigma_{e\epsilon} = \text{cov}(e_{ij}\epsilon_{ij})$ for all i and j, so that $\sigma_{x_{1ij}x_{2ij}} = \sigma_{\alpha\beta} + \sigma_{e\epsilon} \equiv \sigma_{xy}$ for all i and j.

Although for balanced data (having equal numbers of observations in the subclasses) there is a universally acceptable method of estimating variance components, for unbalanced data (having unequal subclass numbers) there are

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many methods of estimation, see Searle [1971] and LaMotte [1973] for example. Most of these methods involve quite complicated functions of the observations. For each method of estimating variance components the question then arises as to what are the corresponding estimates of the associated covariance components when 2 or more variables are involved? For example, if variance components estimates are computed by Henderson's Method 3 how does one compute corresponding estimates of covariance components?

Conceptually the answer is easy. Suppose that estimates of σ^2_α and σ^2_β in (1) are $\hat{\sigma}^2_\alpha = \underline{x}_1'\underline{A}\underline{x}_1$ and $\hat{\sigma}^2_\beta = \underline{x}_2'\underline{A}\underline{x}_2$ where $\underline{A}$ is a symmetric matrix and $\underline{x}_1$ and $\underline{x}_2$ are the vectors of observations on the random variables X_1 and X_2. Then the corresponding estimate of the covariance component is $\hat{\sigma}_{\alpha\beta} = \underline{x}_1'\underline{A}\underline{x}_2$.

Even though the bilinear form $\underline{x}_1'\underline{A}\underline{x}_2$ for $\hat{\sigma}_{\alpha\beta}$ is easy to understand, it may not be easy to calculate using computer programs designed for calculating variance component estimates which are quadratic forms of the nature $\hat{\sigma}^2_\alpha = \underline{x}_1'\underline{A}\underline{X}_1$ and $\hat{\sigma}^2_\beta = \underline{x}_2'\underline{A}\underline{x}_2$. This is so because programs for computing variance components estimates seldom use the structure of quadratic forms (preferring, instead, a variety of "sums of squares" analogies) and even if they did they could not then readily be used for computing bilinear forms. In contrast, programs for bilinear forms can be used for quadratic forms but they are a little more complex to prepare and few of them exist since, in practice, estimates of variance components are required much more often than are those of covariance components. Designing programs to compute bilinear forms and using them mostly for the special case of quadratic forms would therefore be inefficient. However, because of the identity

$$\underline{x}_1'\underline{A}\underline{x}_2 \equiv \tfrac{1}{2}[(\underline{x}_1 + \underline{x}_2)'\underline{A}(\underline{x}_1 + \underline{x}_2) - \underline{x}_1'\underline{A}\underline{x}_1 - \underline{x}_2'\underline{A}\underline{x}_2] , \tag{2}$$

we have

$$\hat{\sigma}_{\alpha\beta} \equiv \tfrac{1}{2}[\hat{\sigma}^2_{\alpha+\beta} - \hat{\sigma}^2_\alpha - \hat{\sigma}^2_\beta] \tag{3}$$

as used in Rounsaville [1971], where $\hat{\sigma}^2_{\alpha+\beta}$ is the variance component estimate for the random variable $(X_1 + X_2)$. By calculating $\hat{\sigma}^2_{\alpha+\beta}$ from the same computer program that provides $\hat{\sigma}^2_\alpha$ and $\hat{\sigma}^2_\beta$, we then obtain $\hat{\sigma}_{\alpha\beta}$ from (3) without any concern for direct calculation of the bilinear form $\underline{x}_1'\underline{A}\underline{x}_2$. Hence covariance components estimates corresponding to any method of estimating variance components by quadratic forms can be calculated from (3) by calculating variance component estimates of the variables and of their sum.

Result (3) is, of course, analogous to the familiar form $\sigma_{XY} = \frac{1}{2}(\sigma^2_{X+Y} - \sigma^2_X - \sigma^2_Y)$ and so could well be anticipated. Nevertheless, (2) shows that (3) is true universally for all variance components estimators that are quadratic forms. This covers most methods of estimation, no matter what the underlying model is. Specific computational formulae for estimates of covariance are therefore not needed.

Covariance components estimates can be readily calculated from (3) but their sampling variances are best derived from the bilinear form $\hat{\sigma}_{\alpha\beta} = \underline{x}_1'\underline{A}\underline{x}_2$. Under normality, the covariance between any two bilinear forms, e.g., Searle [1971, p. 66], yields

$$v(\hat{\sigma}_{\alpha\beta}) = v(\underline{x}_1'\underline{A}\underline{x}_2) = tr(\underline{A}\underline{C})^2 + tr(\underline{A}\underline{V}_1\underline{A}\underline{V}_2) + 2\underline{\mu}_1'\underline{A}\underline{C}\underline{A}\underline{\mu}_2 + \underline{\mu}_1'\underline{A}\underline{V}_2\underline{A}\underline{\mu}_1 + \underline{\mu}_1'\underline{A}\underline{V}_1\underline{A}\underline{\mu}_2$$

where $\underline{\mu}_1$, $\underline{\mu}_2$ and $\underline{V}_1, \underline{V}_2$ are the vectors of means and variance-covariance matrices of $\underline{x}_1$ and $\underline{x}_2$ respectively, and $\underline{C}$ is the matrix of covariances between elements of $\underline{x}_1$ and those of $\underline{x}_2$. Similarly

$$cov(\hat{\sigma}^2_\alpha, \hat{\sigma}_{\alpha\beta}) = cov(\underline{x}_1'\underline{A}\underline{x}_1, \ \underline{x}_1'\underline{A}\underline{x}_2) = tr(\underline{A}\underline{V}_1\underline{A}\underline{C}) + tr(\underline{A}\underline{V}_1)^2 + 2\underline{\mu}_1'\underline{A}\underline{C}\underline{\mu}_1 + 2\underline{\mu}_1'\underline{A}\underline{V}_1\underline{A}\underline{\mu}_2$$

and

$$cov(\hat{\sigma}^2_\alpha, \hat{\sigma}^2_\beta) = cov(\underline{x}_1'\underline{A}\underline{x}_1. \ \underline{x}_2'\underline{A}\underline{x}_2) = 2tr(\underline{A}\underline{C})^2 + 4\underline{\mu}_1'\underline{A}\underline{C}\underline{A}\underline{\mu}_2 ,$$

along with the familiar

$$v(\hat{\sigma}^2_\alpha) = 2\mathrm{tr}(\underline{A}\underline{V}_1)^2 + 4\underline{\mu}_1'\underline{A}\underline{V}_1\underline{A}\underline{\mu}_1 .$$

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