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Asymptotic Variances of Functions of ML and REML Estimates of Variance and Covariance Components

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Description of the Problem

Assume we have computed $\hat{\theta}$, the MLE of θ, and $\text{var}(\hat{\theta}) = [I(\theta)]^{-1}$, its corresponding asymptotic variance.

We now want to compute $\hat{\phi}$, the MLE of ϕ , and $\text{var}(\hat{\phi}) = [I(\phi)]^{-1}$, its asymptotic variance.

Assume that $\phi = f(\theta)$, and that the inverse transformation is $f^{-1}(\phi) = \theta$. Thus, the MLE of ϕ , by the **invariance property of the MLE**, is $\hat{\phi} = f(\hat{\theta})$.

Derivation of the Asymptotic Variance of $\phi = f(\theta)$

Denote the log-likelihood of the **original variable** θ as $\ell(\theta|y)$. By the chain rule of differentiation, the first derivative of $\ell(\theta|y)$ with respect to ϕ is:

$$\frac{\partial \ell(\theta|y)}{\partial\phi} = \underbrace{\frac{\partial \ell(\theta|y)}{\partial\theta}}_{u}\underbrace{\frac{\partial\theta}{\partial\phi}}_{v}$$

and the second derivative of $\ell(\theta|y)$ with respect to ϕ is:

$$\frac{\partial^2 \ell(\theta|y)}{\partial\phi} = \underbrace{\frac{\partial \ell(\theta|y)}{\partial\theta}}_{u}\underbrace{\frac{\partial^2\theta}{(\partial\phi)^2}}_{dv} + \underbrace{\frac{\partial}{\partial\phi}\left[\frac{\partial \ell(\theta|y)}{\partial\theta}\right]}_{du}\underbrace{\frac{\partial\theta}{\partial\phi}}_{v}$$

The first part of the second term, by the chain rule, is equal to:

$$\frac{\partial}{\partial\phi}\left[\frac{\partial \ell(\theta|y)}{\partial\theta}\right] = \frac{\partial}{\partial\theta}\left[\frac{\partial \ell(\theta|y)}{\partial\theta}\right]\frac{\partial\theta}{\partial\phi} .$$

Thus, the second derivative of $\ell(\theta|y)$ with respect to ϕ is equal to:

$$\frac{\partial^2 \ell(\theta|y)}{\partial\phi^2} = \frac{\partial \ell(\theta|y)}{\partial\theta}\frac{\partial^2\theta}{(\partial\phi)^2} + \frac{\partial^2 \ell(\theta|y)}{(\partial\theta)^2}\left(\frac{\partial\theta}{\partial\phi}\right)^2$$

The expectation of the second derivative of $\ell(\theta|y)$ with respect to ϕ is:

$$E_y\left[\frac{\partial^2 \ell(\theta|y)}{\partial\phi^2}\right] = \underbrace{E_y\left[\frac{\partial\ell(\theta|y)}{\partial\theta}\right]}_{=\ \text{E[Score]}\ =\ 0}\underbrace{\frac{\partial^2\theta}{(\partial\phi)^2}}_{\text{constant w.r.t. y}} + E_y\left[\frac{\partial^2\ell(\theta|y)}{(\partial\theta)^2}\right]\underbrace{\left(\frac{\partial\theta}{\partial\phi}\right)^2}_{\text{constant w.r.t. y}}$$

Thus,

$$\underbrace{(-)E_y\left[\frac{\partial^2\ell(\theta|y)}{(\partial\phi)^2}\right]}_{I(\phi)} = \underbrace{(-)E_y\left[\frac{\partial^2\ell(\theta|y)}{(\partial\theta)^2}\right]}_{I(\theta)}\left(\frac{\partial\theta}{\partial\phi}\right)^2$$

Multiplication of both sides above by -1 yields:

$$I(\phi) = I(\theta)\left(\frac{\partial\theta}{\partial\phi}\right)^2 \quad \begin{array}{l}\leftarrow \text{original variable}\\ \leftarrow \text{transformed variable}\end{array}$$

where $I(\phi)$ = information matrix for ϕ, and $I(\theta)$ = information matrix for θ.

The asymptotic variance of ϕ is obtained by inverting $I(\theta)$. Thus,

$$[I(\phi)]^{-1} = [I(\theta)]^{-1}\left(\frac{\partial\theta}{\partial\phi}\right)^{-2} \quad \begin{array}{l}\leftarrow \text{original variable}\\ \leftarrow \text{transformed variable}\end{array}$$

Because $\phi = f(\theta)$, the second term of the right hand side is equal to:

$$\left(\frac{\partial\theta}{\partial\phi}\right)^{-2} = \frac{\mathbf{1}}{\left(\frac{\partial\phi}{\partial\theta}\right)^{-2}} = \left(\frac{\partial\phi}{\partial\theta}\right)^2$$

Thus, the asymptotic variance of ϕ (scalar) is computed as follows:

$$\text{var}(\phi)\Big|_{\hat\phi} = \text{var}(\theta)\Big|_{\hat\theta}\left(\frac{\partial\phi}{\partial\theta}\right)^2 \quad \begin{array}{l}\leftarrow \text{transformed variable}\\ \leftarrow \text{original variable}\end{array}$$

and the asymptotic variance of ϕ (vector) is equal to:

$$\operatorname{var}(\phi)\Big|_{\hat{\phi}} = \frac{\partial \phi}{\partial \theta}^{T} \operatorname{var}(\theta)\Big|_{\hat{\theta}} \left(\frac{\partial \phi}{\partial \theta}\right) .$$

Define $W = \dfrac{\partial \phi}{\partial \theta}$.

Thus,

$$\operatorname{var}(\phi)\Big|_{\hat{\phi}} = W'\big|_{\hat{\theta}} \operatorname{var}(\theta)\Big|_{\hat{\theta}} W\big|_{\hat{\theta}} ,$$

and the standard error of the MLE of ϕ is the square root of the variance of the MLE of ϕ.

Asymptotic Distributions

$\hat{\theta} \sim N\left(\theta,\ \left(I_n(\theta)\right)^{-1}\right)$, where the sample size n → ∞.

$$\hat{\phi} \sim N(\phi,\ W' \underbrace{(I_n(\theta))^{-1}}_{\operatorname{var}(\hat{\theta})} W)$$

Example 1: Derivation of the variance of the REML estimate of the correlation between 2 variables.

Let the original parameter and its variance be:

$$\theta = \begin{bmatrix} \sigma_{11} \\ \sigma_{12} \\ \sigma_{22} \end{bmatrix} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}, \text{ and } var(\theta) = \begin{bmatrix} \mathrm{var}(\sigma_{11}) & \mathrm{cov}(\sigma_{11}, \sigma_{12}) & \mathrm{cov}(\sigma_{11}, \sigma_{12}) \\ & \mathrm{var}(\sigma_{12}) & \mathrm{cov}(\sigma_{12}\sigma_{22}) \\ Sym. & & \mathrm{var}(\sigma_{22}) \end{bmatrix}.$$

Let the transformed parameter be:

$$\phi = \frac{\sigma_{12}}{\sigma_{11}^{1/2}\sigma_{22}^{1/2}} \quad .$$

The derivative of ϕ with respect to θ is:

$$\frac{\partial\phi}{\partial\theta} = \begin{bmatrix} \frac{\partial\phi}{\partial\sigma_{11}} \\ \frac{\partial\phi}{\partial\sigma_{12}} \\ \frac{\partial\phi}{\partial\sigma_{22}} \end{bmatrix}$$

where, using the formula of the derivative of a ratio, i.e., $\left(\frac{f}{g}\right)' = \frac{gf' - fg'}{g^2}$,

$$\frac{\partial\phi}{\partial\sigma_{11}} = \frac{\partial\left(\frac{\sigma_{12}}{\sigma_{11}^{1/2}\sigma_{22}^{1/2}}\right)}{\partial\sigma_{11}}$$

$$= \frac{\left(\sigma_{11}^{1/2}\sigma_{22}^{1/2}\right)\frac{\partial\sigma_{12}}{\partial\sigma_{11}} - \sigma_{12}\left(\frac{1}{2}\sigma_{11}^{-1/2}\right)}{\sigma_{11}^{1/2}\sigma_{22}^{1/2}}$$

$$= \frac{-\frac{1}{2}\sigma_{11}^{-1/2}\sigma_{12}}{\sigma_{11}\sigma_{22}} = \frac{-\frac{1}{2}\sigma_{12}}{\sigma_{11}^{3/2}\sigma_{22}} \Rightarrow w_1 = \frac{-\frac{1}{2}\hat{\sigma}_{12}}{\hat{\sigma}_{11}^{3/2}\hat{\sigma}_{22}}$$

$$\frac{\partial\phi}{\partial\sigma_{12}} = \frac{\partial\left(\frac{\sigma_{12}}{\sigma_{11}^{1/2}\sigma_{22}^{1/2}}\right)}{\partial\sigma_{12}} = \frac{1}{\sigma_{11}^{1/2}\sigma_{22}^{1/2}} \Rightarrow w_2 = \frac{1}{\hat{\sigma}_{11}^{1/2}\hat{\sigma}_{22}^{1/2}}$$

$$\frac{\partial\phi}{\partial\sigma_{22}} = \frac{\partial\left(\frac{\sigma_{12}}{\sigma_{11}^{1/2}\sigma_{22}^{1/2}}\right)}{\partial\sigma_{22}} = \frac{\left(\sigma_{11}^{1/2}\sigma_{22}^{1/2}\right)\frac{\partial\sigma_{12}}{\partial\sigma_{22}} - \sigma_{12}\left(\frac{1}{2}\sigma_{22}^{-1/2}\right)}{\left(\sigma_{11}^{1/2}\sigma_{22}^{1/2}\right)^2}$$

$$= \frac{-\frac{1}{2}\sigma_{12}\sigma_{22}^{-1/2}}{\left(\sigma_{11}^{1/2}\sigma_{22}^{1/2}\right)^2} = \frac{-\frac{1}{2}\sigma_{12}}{\sigma_{11}\sigma_{22}^{3/2}} \Rightarrow w_3 = \frac{-\frac{1}{2}\hat{\sigma}_{12}}{\hat{\sigma}_{11}\hat{\sigma}_{22}^{3/2}}$$

The variance of the REML estimate of the correlation coefficient between 2 traits is computed using:

$$\mathbf{var}(\phi)\Big|_{\hat{\theta}, \hat{\phi}} = w^T \overbrace{\mathbf{var}(\hat{\theta})}^{(I_n(\phi))^{-1}} w$$

$$\mathbf{var}(\phi)\Big|_{\hat{\theta}, \hat{\phi}} = \begin{bmatrix} w_1 & w_2 & w_3 \end{bmatrix} \underbrace{\begin{bmatrix} v_{\theta_1\theta_1} & v_{\theta_1\theta_2} & v_{\theta_1\theta_3} \\ v_{\theta_2\theta_1} & v_{\theta_2\theta_2} & v_{\theta_2\theta_3} \\ v_{\theta_3\theta_1} & v_{\theta_3\theta_2} & v_{\theta_3\theta_3} \end{bmatrix}\Bigg|_{\hat{\theta}}^{-1}}_{\left[I_n(\theta)\right]^{-1}} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

and the standard error of the REML correlation estimate is:

$$SE(\phi)\Big|_{\theta}^{\hat{\phi}} = SQRT[\text{var}(\phi)]\Big|_{\theta}^{\hat{\phi}} .$$

Example 2: Derivation of the variance of the REML estimate of the heritability of a trait.

Define:

$\sigma_{AA} =$ additive direct genetic variance,
$\sigma_{AM} = \sigma_{MA} =$ additive direct - maternal genetic covariance,
$\sigma_{MM} =$ additive maternal genetic variance, and
$\sigma_{PP} = \sigma_{AA} + \sigma_{AM} + \sigma_{MM} + \sigma_{EE} =$ phenotypic variance.

Let

$$\theta = \begin{bmatrix} \sigma_{AA} \\ \sigma_{AM} \\ \sigma_{MM} \\ \sigma_{EE} \end{bmatrix}$$

$$\phi = \frac{\sigma_{AA}}{\sigma_{PP}}$$

The REML estimate of ϕ is:

$$\hat{\phi} = \frac{\hat{\sigma}_{AA}}{\hat{\sigma}_{AA} + \hat{\sigma}_{AM} + \hat{\sigma}_{MM} + \hat{\sigma}_{EE}} .$$

The variance of the REML estimate of ϕ is:

$$\mathbf{var}\left(\hat{\phi}\right) = w' \,\mathbf{var}\left(\hat{\theta}\right) w ,$$

where

$$w = \frac{\partial\phi}{\partial\theta} = \begin{bmatrix} \frac{\partial\phi}{\partial\sigma_{AA}} \\ \frac{\partial\phi}{\partial\sigma_{AM}} \\ \frac{\partial\phi}{\partial\sigma_{MM}} \\ \frac{\partial\phi}{\partial\sigma_{EE}} \end{bmatrix}$$

Each term in the above vector is obtained using the derivative of a ratio, $\left(\frac{f}{g}\right)' = \frac{gf' - fg'}{g^2}$,

$$\frac{\partial\phi}{\partial\sigma_{AA}} = \frac{\partial\left(\frac{\sigma_{AA}}{\sigma_{PP}}\right)}{\partial\sigma_{AA}} = \frac{(\sigma_{PP})(\mathbf{1}) - (\sigma_{AA})(\mathbf{1})}{(\sigma_{PP})^2}$$

$$= \frac{\sigma_{PP} - \sigma_{AA}}{(\sigma_{PP})^2} \Rightarrow w_1 = \frac{\hat{\sigma}_{PP} - \hat{\sigma}_{AA}}{(\hat{\sigma}_{PP})^2}$$

$$\frac{\partial\phi}{\partial\sigma_{AM}} = \frac{(\sigma_{PP})(0) - (\sigma_{AA})(1)}{(\sigma_{PP})^2}$$

$$= \frac{-\sigma_{AA}}{(\sigma_{PP})^2} \Rightarrow w_2 = \frac{-\hat{\sigma}_{AA}}{(\hat{\sigma}_{PP})^2}$$

$$\frac{\partial\phi}{\partial\sigma_{MM}} = \frac{-\sigma_{AA}}{(\sigma_{PP})^2} \Rightarrow w_3 = \frac{-\hat{\sigma}_{AA}}{(\hat{\sigma}_{PP})^2}$$

$$\frac{\partial\phi}{\partial\sigma_{EE}} = \frac{-\sigma_{AA}}{(\sigma_{PP})^2} \Rightarrow w_4 = \frac{-\hat{\sigma}_{AA}}{(\hat{\sigma}_{PP})^2}$$

Thus, the variance of the REML estimate of the heritability of a trait is equal to:

$$\mathbf{var}\left(\hat{\phi}\right) = \begin{bmatrix} w_1 & w_2 & w_3 & w_4 \end{bmatrix} \underbrace{\left(I_n(\theta)\right)^{-1}}_{\mathbf{var}\left(\hat{\theta}\right)} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix}$$

Example 3: Derivation of the variance of the REML estimates of phenotypic covariances.

Let the genetic and environmental covariances between traits i and j (i = j, or i ≠ j) be:

$$\theta = \begin{bmatrix} \sigma_{A_i A_j} \\ \frac{1}{2}\sigma_{A_i M_j} \\ \frac{1}{2}\sigma_{M_i A_j} \\ \sigma_{M_i M_j} \\ \sigma_{E_i E_j} \end{bmatrix}$$

The phenotypic covariance between traits i and j is:

$$\phi = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{2} & 1 & 1 \end{bmatrix} \begin{bmatrix} \sigma_{A_i A_j} \\ \sigma_{A_i M_j} \\ \sigma_{M_i A_j} \\ \sigma_{M_i M_j} \\ \sigma_{E_i E_j} \end{bmatrix} = w' \theta$$

The REML estimate of the phenotypic covariance between traits i and j is:

$$\hat{\phi} = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{2} & 1 & 1 \end{bmatrix} \begin{bmatrix} \hat{\sigma}_{A_i A_j} \\ \hat{\sigma}_{A_i M_j} \\ \hat{\sigma}_{M_i A_j} \\ \hat{\sigma}_{M_i M_j} \\ \hat{\sigma}_{E_i E_j} \end{bmatrix} = w' \hat{\theta} \quad .$$

The elements of vector w were obtained as follows:

$$w_1 = \frac{\partial\phi}{\partial\sigma_{A_iA_j}} = 1,$$

$$w_2 = \frac{\partial\phi}{\partial\sigma_{A_iM_j}} = \tfrac{1}{2},$$

$$w_3 = \frac{\partial\phi}{\partial\sigma_{M_iA_j}} = \tfrac{1}{2},$$

$$w_4 = \frac{\partial\phi}{\partial\sigma_{M_iM_j}} = 1, \text{ and}$$

$$w_5 = \frac{\partial\phi}{\partial\sigma_{E_iE_j}} = 1.$$

The variance of the REML estimate of the phenotypic covariance between traits i and j is:

$$\operatorname{var}\left(\hat{\phi}\right) = \begin{bmatrix} 1 & \tfrac{1}{2} & \tfrac{1}{2} & 1 & 1 \end{bmatrix} \underbrace{\operatorname{var}\left(\hat{\theta}\right)}_{[I(\theta)]^{-1}} \begin{bmatrix} 1 \\ \tfrac{1}{2} \\ \tfrac{1}{2} \\ 1 \\ 1 \end{bmatrix} = w' \operatorname{var}(\hat{\theta}) w.$$

The covariance matrix of REML estimates of phenotypic covariances among several traits is:

$$\operatorname{var}\left(\hat{\phi}\right) = W' \operatorname{var}\left(\hat{\theta}\right) W$$

where $W = \left\{ w_{ij} \right\}$, i ≥ j = 1, ..., number of traits.

Example 4: Derivation of the variance of the REML estimates of phenotypic correlations.

Consider 3 growth traits: birth weight (BW), weight gain from birth to weaning (BWG), and weight gain from weaning to 550 days of age (WHG).

Step 1. Compute $\operatorname{var}\left(\hat{\sigma}_{P_iP_j}\right)$ using the expression for $\operatorname{var}\left(\hat{\phi}_{ij}\right)$ above, where $\hat{\phi}_{ij}$ = phenotypic covariances between traits i and j, and j ≥ i = 1, 2, 3. The resulting $\mathrm{var}(\hat{\phi})$ matrix has dimension equal to 6 (i.e., ½(3 × 4) = 6).

Step 2. Compute $\mathrm{var}(\hat{\varphi}) = W' \, \mathrm{var}(\hat{\phi}) W$,

where

$$W' = \begin{bmatrix} w_{11} & w_{12} & w_{13} & w_{22} & w_{23} & w_{33} \end{bmatrix}.$$

For any two traits i and j, the weights are :

$$w_{ii} = \frac{-\tfrac{1}{2}\hat{\phi}_{ij}}{\hat{\phi}_{ii}^{\,3/2}\hat{\phi}_{jj}}$$

$$w_{ij} = \frac{1}{\hat{\phi}_{ii}^{\,1/2}\hat{\phi}_{jj}^{\,1/2}}$$

$$w_{jj} = \frac{-\tfrac{1}{2}\hat{\phi}_{ij}}{\hat{\phi}_{ii}^{\,1/2}\hat{\phi}_{jj}^{\,3/2}}$$

where the $\{\hat{\phi}_{ij}\}$ are the **REML estimates of phenotypic variances and covariances**.

The **covariance matrix of the REML estimates of phenotypic variances and covariances** is:

$$\mathrm{var}(\hat{\phi}) = \begin{bmatrix} v(\hat{\phi}_{11}) & c(\hat{\phi}_{11},\hat{\phi}_{12}) & c(\hat{\phi}_{11},\hat{\phi}_{13}) & c(\hat{\phi}_{11},\hat{\phi}_{22}) & c(\hat{\phi}_{11},\hat{\phi}_{23}) & c(\hat{\phi}_{11},\hat{\phi}_{33}) \\ & v(\hat{\phi}_{12}) & c(\hat{\phi}_{12},\hat{\phi}_{13}) & c(\hat{\phi}_{12},\hat{\phi}_{22}) & c(\hat{\phi}_{12},\hat{\phi}_{23}) & c(\hat{\phi}_{12},\hat{\phi}_{33}) \\ & & v(\hat{\phi}_{13}) & c(\hat{\phi}_{13},\hat{\phi}_{13}) & c(\hat{\phi}_{13},\hat{\phi}_{23}) & c(\hat{\phi}_{13},\hat{\phi}_{33}) \\ & & & v(\hat{\phi}_{22}) & c(\hat{\phi}_{22},\hat{\phi}_{23}) & c(\hat{\phi}_{22},\hat{\phi}_{33}) \\ & Sym. & & & v(\hat{\phi}_{23}) & c(\hat{\phi}_{23},\hat{\phi}_{33}) \\ & & & & & v(\hat{\phi}_{33}) \end{bmatrix}$$

For example, the variance of the phenotypic correlation between traits 1 and 2 (e.g., BW, and BWG), is computed as follows:

$$\mathrm{var}\left(\hat{\varphi}_{12}\right) = \overbrace{\begin{bmatrix} w_{11} & w_{12} & 0 & w_{22} & 0 & 0 \end{bmatrix}}^{w'} \mathrm{var}\left(\hat{\phi}\right) \overbrace{\begin{bmatrix} w_{11} \\ w_{12} \\ 0 \\ w_{22} \\ 0 \\ 0 \end{bmatrix}}^{w} .$$

The matrix W for the 3 traits is:

$$W'_{3\times 6} = \begin{bmatrix} w_{11} & w_{12} & 0 & w_{22} & 0 & 0 \\ w_{11} & 0 & w_{13} & 0 & 0 & w_{33} \\ 0 & 0 & 0 & w_{22} & w_{23} & w_{33} \end{bmatrix} ,$$

and the variance of the REML estimates of correlations among the 3 growth traits is:

$$\mathrm{var}\left(\hat{\phi}\right) = W' \,\mathrm{var}\left(\hat{\phi}\right) W .$$

References

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