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 \( \Theta \), and \( \text{var}(\hat{\Theta}) = [I(\Theta)]^{-1} \), its corresponding asymptotic variance.

We now want to compute \( \hat{\phi} \), the MLE of \( \phi \), 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 \( \phi \), 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 \( \Theta \) as \( \ell(\Theta|y) \). By the chain rule of differentiation, the first derivative of \( \ell(\Theta|y) \) with respect to \( \phi \) is:

\[
\frac{\partial \ell(\Theta|y)}{\partial \phi} = \frac{\partial \ell(\Theta|y)}{\partial \Theta} \frac{\partial \Theta}{\partial \phi} + \frac{\partial \ell(\Theta|y)}{\partial \phi}
\]

and the second derivative of \( \ell(\Theta|y) \) with respect to \( \phi \) is:

\[
\frac{\partial^2 \ell(\Theta|y)}{\partial \phi^2} = \frac{\partial \ell(\Theta|y)}{\partial \Theta} \frac{\partial^2 \Theta}{\partial \phi^2} + \frac{\partial \ell(\Theta|y)}{\partial \phi} \frac{\partial \Theta}{\partial \phi}
\]

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 \( \phi \) is equal to:

\[
\frac{\partial^2 \ell(\Theta|y)}{\partial \phi^2} = \frac{\partial \ell(\Theta|y)}{\partial \Theta} \frac{\partial^2 \Theta}{\partial \phi^2} + \frac{\partial \ell(\Theta|y)}{\partial \phi} \frac{(\partial \Theta)^2}{(\partial \phi)^2}
\]
The expectation of the second derivative of $\ell(\theta|y)$ with respect to $\phi$ is:

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

$$
= E[\text{Score}] = 0 \quad \text{constant} \quad \text{w.r.t. } y
$$

Thus,

$$
(-1) E_y\left[\frac{\partial^2 \ell(\theta|y)}{(\partial \phi)^2}\right] = (-1) E_y\left[\frac{\partial^2 \ell(\theta|y)}{(\partial \theta)^2}\right] \left(\frac{\partial \theta}{\partial \phi}\right)^2
$$

$$
I(\phi) = I(\theta) \left(\frac{\partial \theta}{\partial \phi}\right)^2 \quad \text{original variable}
$$

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

Thus, the asymptotic variance of $\phi$ (scalar) is computed as follows:

$$
\text{var}(\phi|_{\phi}) = \text{var}(\theta|_{\phi}) \left(\frac{\partial \phi}{\partial \theta}\right)^2 \quad \text{transformed variable}
$$

$$
\text{var}(\theta|_{\phi}) \left(\frac{\partial \phi}{\partial \theta}\right)^2 \quad \text{original variable}
$$
and the asymptotic variance of $\phi$ (vector) is equal to:

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

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

Thus,

$$\text{var}(\phi)|_{\hat{\theta}} = W^T|_{\hat{\theta}} \text{var}(\theta)|_{\hat{\theta}} W|_{\hat{\theta}},$$

and the standard error of the MLE of $\phi$ is the square root of the variance of the MLE of $\phi$.

**Asymptotic Distributions**

$$\hat{\theta} \sim N\left(\theta, \left(I_n(\theta)\right)^{-1}\right),$$

where the sample size $n \to \infty$.

$$\hat{\phi} \sim N(\phi, \frac{W^T(I_n(\theta))^{-1}W}{\text{var}(\hat{\theta})})$$
Example 1: Derivation of the variance of the REML estimate of the correlation between 2 variables.

Let the original parameter and its variance be:

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

Let the transformed parameter be:

\[
\phi = \frac{\sigma_{12}}{\sigma_{11}^{1/2} \sigma_{22}^{1/2}}.
\]

The derivative of \( \phi \) with respect to \( \theta \) 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., \( \left( \frac{f}{g} \right)' = \frac{gf' - fg'}{g^2} \),

\[
\frac{\partial \phi}{\partial \sigma_{11}} = \left( \frac{\sigma_{12}}{\sigma_{11}^{1/2} \sigma_{22}^{1/2}} \right) \frac{\partial}{\partial \sigma_{11}} \left( \frac{\sigma_{12}}{\sigma_{11}^{1/2} \sigma_{22}^{1/2}} \right)
\]
The variance of the REML estimate of the correlation coefficient between 2 traits is computed using:

\[
\text{var}(\phi) \bigg|_{\hat{\theta}} = \mathbf{w}^T \text{var}(\hat{\theta}) \mathbf{w}
\]

\[
\text{var}(\phi) \bigg|_{\hat{\theta}} = \begin{pmatrix} w_1 & w_2 & w_3 \end{pmatrix} \begin{bmatrix}
\gamma_{\theta_1, \theta_1} & \gamma_{\theta_1, \theta_2} & \gamma_{\theta_1, \theta_3} \\
\gamma_{\theta_2, \theta_1} & \gamma_{\theta_2, \theta_2} & \gamma_{\theta_2, \theta_3} \\
\gamma_{\theta_3, \theta_1} & \gamma_{\theta_3, \theta_2} & \gamma_{\theta_3, \theta_3}
\end{bmatrix}^{-1} \begin{pmatrix} w_1 \\
w_2 \\
w_3 \end{pmatrix}
\]
and the standard error of the REML correlation estimate is:

\[ SE(\hat{\phi}) = \sqrt{\text{var}(\hat{\phi})} \]  

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

Define:

\[ \sigma_{AA} = \text{additive direct genetic variance}, \]
\[ \sigma_{AM} = \sigma_{MA} = \text{additive direct - maternal genetic covariance}, \]
\[ \sigma_{MM} = \text{additive maternal genetic variance}, \]
\[ \sigma_{PP} = \sigma_{AA} + \sigma_{AM} + \sigma_{MM} + \sigma_{BB} = \text{phenotypic variance}. \]

Let

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

\[ \phi = \frac{\sigma_{AA}}{\sigma_{PP}} \]

The REML estimate of \( \phi \) 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 \( \phi \) is:

\[ \text{var}(\hat{\phi}) = w' \text{var}(\hat{\theta}) w, \]

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

\[
\frac{\partial \phi}{\partial \sigma_{AA}} = \frac{\partial \left( \frac{\sigma_{AA}}{\sigma_{PP}} \right)}{\partial \sigma_{AA}} = \frac{(\sigma_{PP})(1) - (\sigma_{AA})(1)}{(\sigma_{PP})^2} = \frac{\sigma_{PP} - \sigma_{AA}}{(\sigma_{PP})^2} \Rightarrow W_1 = \frac{\hat{\sigma}_{PP} - \hat{\sigma}_{AA}}{(\hat{\sigma}_{PP})^2}
\]

\[
\frac{\partial \phi}{\partial \sigma_{AM}} = \frac{(\partial \sigma_{PP}) - (\sigma_{AA})(1)}{(\sigma_{PP})^2} = \frac{-\sigma_{AA}}{(\sigma_{PP})^2} \Rightarrow W_2 = \frac{-\hat{\sigma}_{AA}}{(\hat{\sigma}_{PP})^2}
\]

\[
\frac{\partial \phi}{\partial \sigma_{MM}} = \frac{-\sigma_{AA}}{(\sigma_{PP})^2} \Rightarrow W_3 = \frac{-\hat{\sigma}_{AA}}{(\hat{\sigma}_{PP})^2}
\]

\[
\frac{\partial \phi}{\partial \sigma_{EE}} = \frac{-\sigma_{AA}}{(\sigma_{PP})^2} \Rightarrow W_4 = \frac{-\hat{\sigma}_{AA}}{(\hat{\sigma}_{PP})^2}
\]

Thus, the variance of the REML estimate of the heritability of a trait is equal to:
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 $i \neq j$) be:

$$
\Theta = \begin{bmatrix}
\sigma_{AA}, \\
\frac{1}{2} \sigma_{AM}, \\
\frac{1}{2} \sigma_{MA}, \\
\sigma_{MM}, \\
\sigma_{EE},
\end{bmatrix}
$$

The phenotypic covariance between traits $i$ and $j$ is:

$$
\phi = \begin{bmatrix}
1 & \frac{1}{2} & \frac{1}{2} & 1
\end{bmatrix}
\begin{bmatrix}
\sigma_{AA} \\
\sigma_{AM} \\
\sigma_{MA} \\
\sigma_{MM}
\end{bmatrix} = \phi' \Theta
$$

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

$$
\hat{\phi} = \begin{bmatrix}
1 & \frac{1}{2} & \frac{1}{2} & 1
\end{bmatrix}
\begin{bmatrix}
\hat{\sigma}_{AA} \\
\hat{\sigma}_{AM} \\
\hat{\sigma}_{MA} \\
\hat{\sigma}_{MM}
\end{bmatrix} = \phi' \hat{\Theta}
$$
The elements of vector \( w \) were obtained as follows:

\[
\begin{align*}
\omega_1 &= \frac{\partial \phi}{\partial \sigma_{a,i}} = 1, \\
\omega_2 &= \frac{\partial \phi}{\partial \sigma_{a,j}} = \frac{1}{2}, \\
\omega_3 &= \frac{\partial \phi}{\partial \sigma_{m,i}} = \frac{1}{2}, \\
\omega_4 &= \frac{\partial \phi}{\partial \sigma_{m,j}} = 1, \text{ and} \\
\omega_5 &= \frac{\partial \phi}{\partial \sigma_{g_{i,j}}} = 1.
\end{align*}
\]

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

\[
\text{var}(\hat{\phi}) = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{2} & 1 \end{bmatrix} \text{var}(\hat{\theta}) \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 1 \\ 1 \end{bmatrix} = w' \text{var}(\hat{\theta})w.
\]

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

\[
\text{var}(\hat{\phi}) = W' \text{var}(\hat{\theta})W
\]

where \( W = \left\{ w_{ij} \right\} \), \( i \geq j = 1, \ldots, \text{number of traits} \).

**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 \( \text{var}(\hat{\sigma}_{P,P}) \) using the expression for \( \text{var}(\hat{\phi}_g) \) above, where \( \hat{\phi}_g = \text{phenotypic} \).
covariances between traits i and j, and j \geq i = 1, 2, 3. The resulting $\text{var}(\hat{\phi})$ matrix has
dimension equal to 6 (i.e., $\frac{1}{2}(3 \times 4) = 6$).

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

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:

\[
\begin{align*}
\omega_{ii} & = -\frac{1}{2} \frac{\hat{\phi}_{ii}}{\hat{\phi}_{ii}^2} \\
\omega_{ij} & = 1 - \frac{\hat{\phi}_{ij}}{\hat{\phi}_{ii} \hat{\phi}_{jj}} \\
\omega_{jj} & = -\frac{1}{2} \frac{\hat{\phi}_{jj}}{\hat{\phi}_{jj}^2}
\end{align*}
\]

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:

\[
\text{var}(\hat{\phi}) = \begin{bmatrix}
    \nu(\hat{\phi}_{11}) & c(\hat{\phi}_{11}, \hat{\phi}_{12}) & c(\hat{\phi}_{11}, \hat{\phi}_{13}) & c(\hat{\phi}_{11}, \hat{\phi}_{22}) & c(\hat{\phi}_{11}, \hat{\phi}_{23}) & c(\hat{\phi}_{11}, \hat{\phi}_{33}) \\
    c(\hat{\phi}_{12}, \hat{\phi}_{11}) & \nu(\hat{\phi}_{12}) & c(\hat{\phi}_{12}, \hat{\phi}_{13}) & c(\hat{\phi}_{12}, \hat{\phi}_{22}) & c(\hat{\phi}_{12}, \hat{\phi}_{23}) & c(\hat{\phi}_{12}, \hat{\phi}_{33}) \\
    c(\hat{\phi}_{13}, \hat{\phi}_{11}) & c(\hat{\phi}_{13}, \hat{\phi}_{12}) & \nu(\hat{\phi}_{13}) & c(\hat{\phi}_{13}, \hat{\phi}_{22}) & c(\hat{\phi}_{13}, \hat{\phi}_{23}) & c(\hat{\phi}_{13}, \hat{\phi}_{33}) \\
    c(\hat{\phi}_{22}, \hat{\phi}_{11}) & c(\hat{\phi}_{22}, \hat{\phi}_{12}) & c(\hat{\phi}_{22}, \hat{\phi}_{13}) & \nu(\hat{\phi}_{22}) & c(\hat{\phi}_{22}, \hat{\phi}_{23}) & c(\hat{\phi}_{22}, \hat{\phi}_{33}) \\
    c(\hat{\phi}_{23}, \hat{\phi}_{11}) & c(\hat{\phi}_{23}, \hat{\phi}_{12}) & c(\hat{\phi}_{23}, \hat{\phi}_{13}) & c(\hat{\phi}_{23}, \hat{\phi}_{22}) & \nu(\hat{\phi}_{23}) & c(\hat{\phi}_{23}, \hat{\phi}_{33}) \\
    c(\hat{\phi}_{33}, \hat{\phi}_{11}) & c(\hat{\phi}_{33}, \hat{\phi}_{12}) & c(\hat{\phi}_{33}, \hat{\phi}_{13}) & c(\hat{\phi}_{33}, \hat{\phi}_{22}) & c(\hat{\phi}_{33}, \hat{\phi}_{23}) & \nu(\hat{\phi}_{33})
\end{bmatrix}
\]

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

$$\text{var}(\hat{\phi}) = W' \text{var}(\hat{\phi}) W.$$

References
