

ESTIMATION OF BIVARIATE VARIANCE COMPONENTS

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SUMMARY

The use of derivative-free methods to give maximum likelihood estimates of bivariate variance parameters is illustrated. An algorithm is given for the case when the same fixed effect model applies to both traits and the variance matrices for the two traits and the covariance matrix between the two traits have the same structure. Each of these three matrices depending on two variance parameters, giving a total of six parameters. By reparameterising in terms of canonical heritabilities and a transformation matrix a six dimensional problem is reduced to a two-dimensional problem. Extensions to other models are briefly indicated. One important case is when each animal is measured on only one trait.

INTRODUCTION

With the advances in compute technology it is becoming more practical to predict breeding values using multivariate individual animal models. There is an increasing need to have estimates of variance and covariance parameters for these models. Maximum likelihood techniques (ML or REML) have been advocated as they use all the available information and can take account of known selection decisions as in selection experiments (Henderson *et al.*, 1969) and are less biased than analysis of variance techniques when the selection decisions are not fully known (Meyer and Thompson, 1984).

Estimation in multivariate cases has mimicked univariate methods in using methods that have used first and second differentials of the log-likelihood. These calculations can be expressed in terms of the mixed model equations (Henderson, 1973) and the inverse of this set of equations. As the number of traits increase so do the number of equations. In some cases the equations can be simplified using a canonical transformation (Meyer, 1985) or a Choleski transformation to make the residual covariances zero (as in Henderson *et al.*, 1959). Recently, the advantages of ML methods based on derivative-free approaches have been shown (Graser *et al.*, 1987, Meyer, 1989) for univariate analyses.

We consider an extension to two variates. First for the case when both traits are measured on all animals and the same fixed and random model holds for both traits. We assume there are two random effects associated with each trait giving rise to four variance and two covariance parameters, a total of six parameters. In the analogous univariate case the optimization of two parameters, e.g. genetic and residual variance, can be reduced to a one-dimensional search because the residual variance can be easily found for a given value of heritability. We suggest an analogous decomposition of the six parameters into a 2×2 transformation matrix that makes the traits independent, both genetically and phenotypically, and two canonical heritabilities of the independent traits. It is shown how to derive the

estimate of the transformation matrix given the values for the canonical heritabilities. Maximization is then only over the two dimensions of canonical heritabilities.

METHOD

Let the model for the i th ($i = 1, 2$) trait be

$$y_i = Xb_i + Za_i + e_i$$

where

y_i is a $N \times 1$ vector of observations,
 b_i is a $t \times 1$ vector of unknown fixed effects
 a_i is a $s \times 1$ vector of additive genetic effects, and
 e_i is a $N \times 1$ vector of residual.

The matrices X and Z are $N \times t$ and $N \times s$ matrices that link effects to y_i with X of rank t . It is assumed

$E(y_i) = Xb_i$, $E(a_i) = E(e_i) = 0$
 $\text{Var}(a_i) = \sigma_{A_i}^2 A$, $\text{Var}(e_i) = I\sigma_{e_i}^2$ and $\text{cov}(a_i, e_i) = 0$ and
 $\text{Cov}(a_1, a_2) = \sigma_{A_{12}} A$, $\text{cov}(e_1, e_2) = I\sigma_{E_{12}}$ and $\text{cov}(a_1, e_2) = 0$.

$$\text{Let } \begin{bmatrix} \sigma_{A1}^2 & \sigma_{A12} \\ \sigma_{A12} & \sigma_{A2}^2 \end{bmatrix} = G \text{ and } \begin{bmatrix} \sigma_{E1}^2 & \sigma_{E12} \\ \sigma_{E12} & \sigma_{E2}^2 \end{bmatrix} = R$$

We wish to calculate the residual likelihood, L , associated with error contrasts of y_1 and y_2 for a given value of R and G . Suppose

$$R = TT', \text{ and } G = T \begin{bmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{bmatrix} T' \text{ and } U = T^{-1}$$

$$\text{and } y_{u1} = u_{11} y_1 + u_{12} y_2$$

$$y_{u2} = u_{21} y_1 + u_{22} y_2$$

The traits y_{u1} and y_{u2} are then independent with variance $H_i = I + ZAZ' \gamma_i$ and with the total likelihood of error contrasts, L , satisfies

$$2L = 2L_{u1} + 2L_{u2} - (n-t) \log |TT'|$$

where L_{ui} is the likelihood associated with y_{ui} .

If we define

then L_{ui} can be found from repeated Gaussian elimination on M_i (Smith and Graser, 1986) using

$$M_1 = \begin{bmatrix} Y'Y & Y'X & Y'Z \\ X'Y & X'X & Z'Z \\ Z'Y & Z'X & Z'Z + A^{-1}\gamma_1^{-1} \end{bmatrix} = \begin{bmatrix} Y'Y & F \\ F' & C_1 \end{bmatrix}$$

$$L_{\omega} = \text{const} - \log |C_1| - y_{\omega}' P_1 y_{\omega} - s \log(\gamma_1) \quad (2)$$

where $P_1 = H_1^{-1} - H_1^{-1} X (X'H_1^{-1}X)^{-1} X'H_1^{-1}$.

Then $\log |C_1|$ is the sum of the logs of the pivots when the rows associated with X and Z are eliminated. The sum of squares of residuals $y_{\omega}' P_1 y_{\omega}$ can be found by using $Y = (y_1, y_2)$ in (1) and finding the (2x2) residual matrix W_1 . Then $y_{\omega}' P_1 y_{\omega} = (u_1, u_2)' W_1 (u_1, u_2)$.

For any pair of values of γ_1 and γ_2 $|C_1|$, $|C_2|$, W_1 and W_2 can be calculated and the L for any pair of linear combinations of traits defined by a 2x2 matrix U. The maximum likelihood estimate of U can be found (Juga and Thompson, 1990) by considering

$$y_{\omega} = S_i [\cos \theta_i (C_{11}y_1 + C_{12}y_2) + \sin \theta_i (C_{21}y_1 + C_{22}y_2)].$$

This transformation involves three stages forming linear combination of traits depending on C_{ij} . Secondly a rotation of axes using θ_i and finally scaling using S_i . If C is chosen so that the off-diagonals are zero then it is found that the maximum corresponds to a null rotation ($\theta_1 = 0, \theta_2 = \pi/2$). It is found that

$$y_{\omega 1} = \sqrt{[(N-t)]} (C_{11}y_1 + C_{12}y_2)$$

$$y_{\omega 2} = \sqrt{[(N-t)/d_2]} (C_{21}y_1 + C_{22}y_2)$$

where C contains the elements C_{ij} and satisfies $C W_1 C' = I$ and $C W_2 C' = D$ with D a diagonal matrix with elements d_1, d_2 and $d_1 > d_2$.

Optimization of γ_1 and γ_2 can be carried out using a derivative-free method such as the method of approximating the likelihood using a quadratic approximation. Note that for calculations of likelihood associated with c different canonical heritabilities canonical traits, c^2 likelihoods can be calculated from each pair of canonical traits. Because the likelihood is symmetric in γ_1 and γ_2 it is perhaps useful to parameterize in terms of $(\gamma_1 + \gamma_2)/2$ and $(\gamma_1 - \gamma_2)/2$ and restrict $(\gamma_1 - \gamma_2)/2$ to be positive.

DISCUSSION

This note has presented a very specific method to aid in estimation of bivariate parameters. Meyer (1990) has considered more general multivariate models with p traits and more components. For two components her procedure is equivalent to optimization of a p x p transformation by derivative-free methods for specific values of canonical heritabilities. The method in this paper might suggest improved starting values for her iterative procedure by considering pairs of traits. For estimating three component matrices (R, G_1 and G_2) a transformation usually does not exist to simultaneously diagonalise these three matrices, and so the traits cannot be transformed to independence. But it might be computationally

attractive to maximise parameters over the restricted space such that $R = TT'$, $G_1 = TD_1T'$, $G_2 = TD_2T'$, with D_1 and D_2 diagonal, because this is much easier computationally and might be close to the unrestricted estimate.

When D_1 and D_2 are not diagonal the maximum likelihood of T is the solution of another eigenvalue problem (Thompson, in prep.), based on using a 4×4 residual matrix using Y containing 4 vectors of length the total number of observations and

$$Y = \begin{bmatrix} y_1 & y_2 & 0 & 0 \\ 0 & 0 & y_1 & y_2 \end{bmatrix} \text{ and } X = \begin{bmatrix} X & 0 \\ 0 & X \end{bmatrix}.$$

Another model that fits this general framework is when there are different fixed models for two traits and only one trait is measured on each animal, so that there is no environmental correlation between traits. For example for traits measured in different sexes or environments (Schaeffer *et al.*, 1978). In this case the algorithm of Meyer (1989) which allows estimation of two genetic variances and their covariance can be used, with Y in (2) now containing two vectors of length the total number of observations and

$$Y = \begin{bmatrix} y_1 & 0 \\ 0 & y_2 \end{bmatrix} \quad X = \begin{bmatrix} X_1 & 0 \\ 0 & X_2 \end{bmatrix}$$

An iterative technique can be used to quickly find the residual variances for given scaled genetic variances $R^{-1/2}GR^{-1/2}$ from a residual matrix W .

This idea of extending the Y vector can be useful for multivariate data when the same model holds for all traits but some animals are culled before traits can be measured (Garrick, 1988).

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