

Variance Components Estimation

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- > Including a new trait in a breeding program always starts with estimation of variance components
- > Goal: split the observable variation in phenotypic observations into their source according to the model that we want to use in our evaluations
- > Need to determine a model:
 - * fixed linear effect models: sources of variation: random residuals
 - * mixed linear effect models: sources of variation: residuals, breeding values \Rightarrow genetic additive variance σ_u^2

Why

- ▶ Predictions of breeding values using BLUP requires variance components σ_u^2 or σ_s^2 and σ_e^2
- ▶ So far we have assumed that they are known
- ▶ In reality: must be estimated from data

Sire Model

- ▶ Start with a simple sire model

$$y = X\beta + Z_s s + e$$

with $\text{var}(e) = R$, $\text{var}(s) = A_s \sigma_s^2$ and $\text{var}(y) = Z_s A_s Z_s^T \sigma_s^2 + R$

- ▶ A_s : numerator relationship for sires
- ▶ σ_s^2 corresponds to $0.25 * \sigma_u^2$
- ▶ $R = I * \sigma_e^2$

→ estimate σ_s^2 and σ_e^2 from data

Analysis of Variance (ANOVA)

Principle: Decomposition of sum of squares into the different source, and source are determined by the model

Sources of variation are all components that are present in a model

Why sum of squares? Fixed linear effect model: residual variance estimate is based on the sum of the square residuals.

Source	Degrees of Freedom (<i>df</i>)	Sums of Squares (<i>SSQ</i>)
Overall (μ)	$\text{Rank}(X) = 1$	$y^T X (X^T X)^{-1} X^T y = F$
Sires (s)	$\text{Rank}(Z_s) - \text{Rank}(X) = q - 1$	$y^T Z_s (Z_s^T Z_s)^{-1} Z_s^T y - y^T X (X^T X)^{-1} X^T y = S$
Residual (e)	$n - \text{Rank}(Z_s) = n - q$	$y^T y - y^T Z_s (Z_s^T Z_s)^{-1} Z_s^T y = R$
Total	n	$y^T y$

Sums of Squares

$$F = y^T X(X^T X)^{-1} X^T y = \frac{1}{n} \left[\sum_{i=1}^n y_i \right]^2$$

$$S = y^T Z_s(Z_s^T Z_s)^{-1} Z_s^T y - y^T X(X^T X)^{-1} X^T y = \sum_{i=1}^q \frac{1}{n_i} \left[\sum_{j=1}^{n_i} y_{ij} \right]^2 - F$$

$$R = y^T y - y^T Z_s(Z_s^T Z_s)^{-1} Z_s^T y \stackrel{-F}{=} \sum_{i=1}^n y_i^2 - S - F$$

Estimates

Estimates of variance components σ_e^2 and σ_s^2 are obtained by replacing expected values of S and R by their observed values and by replacing the variance components by their estimates

- ▶ β and s fixed
- ▶ Estimates of σ_e^2 and σ_s^2 are based on observed sums of squares S and R
- ▶ Set their expected values equal to the observed sums of squares

$$E(R) = (n - q)\sigma_e^2$$

$$R = (n - q) \cdot \hat{\sigma}_e^2 \implies \hat{\sigma}_e^2 = R / (n - q)$$

$$E(S) = (q - 1)\sigma_e^2 + \text{tr}(Z_s M Z_s)\sigma_s^2$$

where $M = I - X(X^T X)^{-1}X^T$ and q is the number of sires.

$$\rightarrow \hat{\sigma}_e^2 = \frac{R}{n - q} \text{ and } \hat{\sigma}_s^2 = \frac{S - (q - 1)\hat{\sigma}_e^2}{\text{tr}(Z_s M Z_s)}$$

Numerical Example

Table 1: Small Example Dataset for Variance Components Estimation Using a Sire Model

Animal	Sire	WWG
4	2	2.9
5	1	4.0
6	3	3.5
7	2	3.5

► Model

$$y_{ij} = \mu + s_j + e_i$$

Design Matrices

$$X = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, Z_s = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

ANOVA

An analysis of variance can be constructed as

Source	Degrees of Freedom (df)	Sums of Squares (SSQ)
Overall (μ)	$Rank(X) = 1$	$F = 48.3025$
Sires (s)	$Rank(Z_s) - Rank(X) = q - 1$	$S = 0.4275$
Residual (e)	$n - Rank(Z_s) = n - q$	$R = 0.18$

Estimates

$$M = \begin{bmatrix} 0.75 & -0.25 & -0.25 & -0.25 \\ -0.25 & 0.75 & -0.25 & -0.25 \\ -0.25 & -0.25 & 0.75 & -0.25 \\ -0.25 & -0.25 & -0.25 & 0.75 \end{bmatrix}$$

$$Z_s^T M Z_s = \begin{bmatrix} 0.75 & -0.5 & -0.25 \\ -0.5 & 1 & -0.5 \\ -0.25 & -0.5 & 0.75 \end{bmatrix}$$

Results

$$\hat{\sigma}_e^2 = R = 0.18$$

$$\hat{\sigma}_s^2 = \frac{S - (q - 1)\hat{\sigma}_e^2}{\text{tr}(Z_s^T M Z_s)} = \frac{0.4275 - 2 * 0.18}{2.5} = 0.027$$

Anova in R

- Assume dataset is stored in dataframe called `tbl_num_ex_chp12`

```
tbl_num_ex_chp12$Sire <- as.factor(tbl_num_ex_chp12$Sire)
aov_result <- aov(WWG ~ Sire, data = tbl_num_ex_chp12)
summary(aov_result)
```

		Df	Sum Sq	Mean Sq	F value	Pr(>F)
## Sire		2	0.4275	0.2137	1.187	0.544
## Residuals		1	0.1800	0.1800		

Problem with ANOVA: In certain datasets, estimates of variance components can get negative and they are therefore not valid, because variance components must be non-negative.

Likelihood

- Definition of likelihood

$$L(\mu, \Sigma) = f(y|\mu, \Sigma)$$

Conditional density of the observations y given the parameter μ and Σ . Very often the density f is taken to be a normal distribution, then μ is the mean and Σ is the variance.

with

$$f_Y(y|\mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^n \det(\Sigma)}} \exp \left\{ -\frac{1}{2} (y - \mu)^T \Sigma^{-1} (y - \mu) \right\}$$

multivariate normal distribution

Central Limit Theorem: the distribution of the sum of very many very small effects will converge to a normal distribution.

Infinitesimal model: genetic additive effects (small, many)

Maximum Likelihood

- ▶ Maximize $L(\mu, \Sigma)$ with respect to Σ

$$\hat{\Sigma} = \operatorname{argmax}_{\Sigma} L(\mu, \Sigma)$$

Bayesian Approach

- ▶ Estimates of unknown quantity Σ based on posterior distribution of unknowns given knowns
- ▶ Using Bayes Theorem:

$$\begin{aligned}f(\Sigma|y) &= \frac{f(\Sigma, y)}{f(y)} \\&= \frac{f(y|\Sigma)f(\Sigma)}{f(y)} \\&\propto f(y|\Sigma)f(\Sigma)\end{aligned}$$

where $f(\Sigma)$: prior distribution and $f(y|\Sigma)$: likelihood

Bayesian Estimates

- ▶ Fixed Linear Model with $\Sigma = \begin{bmatrix} \sigma_s^2 \\ \sigma_e^2 \end{bmatrix}$
- ▶ Full conditional distributions
 - ▶ sire variance: $f(\sigma_s^2 | \sigma_e^2, y)$ has a given standard distribution
 - ▶ residual variance: $f(\sigma_e^2 | \sigma_s^2, y)$ has a given standard distribution
- ▶ Draw random numbers from full conditional distributions in turn
- ▶ Result will be samples from posterior distribution
- ▶ Estimates are computed as empirical means and standard deviation based on the samples, e.g for σ_s^2

$$\widehat{\sigma_s^2}_{Bayes} = \frac{1}{N} \sum_{t=1}^N (\sigma_s^2)^{(t)}$$