

- $X = [1, X_c] \quad 1' X_c = 0$
  - $I = \bar{J} + H_c + I - H$
  - $H = X(X'X)^{-1}X' = \bar{J} + H_c$
  - $X = [1, X_1, \dots, X_m]$
  - $I = \bar{J} + H_1 + \dots + H_m + (I - H)$
  - $H_j = R_j(R_j' R_j)^{-1}R_j' - R_{j-1}(R_{j-1}' R_j)^{-1}R_j'$   
 $= X_j(X_j' X_j)^{-1}X_j' \quad \text{if } X_i' X_j = 0 \quad i \neq j$
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The model  $Y = X\beta + \epsilon$  in the complete balanced factorial design

$Y \sim N_n(\mu, \Sigma)$  where  $\mu$  and  $\Sigma$  are determined by the design

e.g. balanced complete blocks with reps.

$$Y_{ijk} = \mu_j + \beta_i + \beta_{ij} + \epsilon_{ijk}$$

$$\mu = 1_b \otimes (\mu_1, \dots, \mu_r)' \otimes 1_r$$

What is the  $X$ -matrix?

Write  $X$  as a Kronecker product

- Put a 1-vector in the position of random factors
- Put a non-singular matrix in the position of fixed factors; eg the identity

$$\text{eg. RCBID} \quad X = I_b \otimes I_t \otimes I_r$$

$$\begin{aligned} X\beta &= (I_b \otimes I_t \otimes I_r)(\beta_1, \dots, \beta_t)' \\ &= (I_b \otimes I_t \otimes I_r)(1 \otimes (\gamma \otimes 1)) \\ &= I_b \otimes (\beta_1, \dots, \beta_t)' \otimes I_r \end{aligned}$$

$$\text{In this case } \beta_j = \mu_j$$

What if  $I_t$  is replaced by the Helmert?

$$X = I_b \otimes P \otimes I_r$$

$$X\beta = I_b \otimes P\beta \otimes I_r$$

$$\text{So } P\beta = (\mu_1, \dots, \mu_t)'$$

$$\beta = P'(\mu_1, \dots, \mu_t)'$$

$$\beta_1 = \sum_{j=1}^t \mu_j / \sqrt{t}$$

$$\beta_2 = (\mu_1 - \mu_2) / \sqrt{2}$$

$$\beta_3 = (\mu_1 + \mu_2 - 2\mu_3) / \sqrt{6} \quad \text{etc.}$$

Q. What matrix  $P$  results in

$$\beta_i = \bar{\mu} \text{ and } \beta_j = \mu_j - \bar{\mu}$$

is the sum constraint parameterization?

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The  $y = X\beta + E$  implies that  $\mu$  lies in the col. space of  $X$  b/c  $\mu = X\beta$

$$C(X) = \{y : y \in X\beta, \beta \in \mathbb{R}^p\}$$

If  $P$   $p \times p$  is nonsingular then

$$X\beta = (X\beta)(P^{-1}\beta) = X^*\delta$$

$$\begin{aligned} \text{But } C(X) &= \{y : y = XPP^{-1}\beta, \beta \in \mathbb{R}^p\} \\ &= \{y : y = X^*\delta, \delta \in \mathbb{R}^p\} \\ &= C(X^*) \end{aligned}$$

The models

$$Y = X\beta + E \quad \text{and} \quad Y = X^*\delta + E$$

are equivalent! Both say  $\mu$  is in  $C(X) = C(X^*)$

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$$RCBD \quad Y = X\beta + E$$

$$\mu = I_b \otimes (\mu_1, \dots, \mu_r)' \otimes I_r$$

$$\underline{E} = (I_b \otimes I_r \otimes I_r) \underline{B} \quad \underline{B} \sim N_b(0, \sigma_B^2 I_b)$$

$$\begin{aligned}
 & + (I_b \otimes I_t \otimes I_r) \tilde{B}^e \quad \tilde{B}^e \sim N_{btr}(0, \sigma_e^2 I_{btr}) \\
 & + (I_b \otimes I_t \otimes I_r) \tilde{R}(\tilde{B}^e) \\
 & \quad R(B^e) \sim N_{btr}(0, \sigma_e^2 I)
 \end{aligned}$$

The general form of a variance components mixed model is

$$Y = X\beta + \sum_{i=1}^q Z_i \tilde{U}_i + \tilde{\varepsilon}$$

where  $Z_i$  is  $n \times c_i$  with rows that are indicator vectors

$$\tilde{U}_i \sim N_{c_i}(0, \sigma_i^2 I_{c_i})$$

$$\tilde{\varepsilon} \sim N_n(0, \sigma^2 I_n)$$

If we set  $\tilde{U}_0 = \tilde{\varepsilon}$ ,  $Z_0 = I_n$  and  $\sigma^2 = \sigma_0^2$

then

$$Y = X\beta + \sum_{i=0}^q Z_i \tilde{U}_i$$


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The general linear mixed model is

$$Y = X\beta + ZU + \tilde{\varepsilon}$$

$$U \sim N(0, D) \quad \tilde{\varepsilon} \sim N(0, G)$$


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For the VC model

$$\mathbf{y} \sim N_n(\mathbf{x}\beta, \Sigma), \quad \Sigma = \sum_{i=0}^q \sigma_i^2 \mathbf{z}_i \mathbf{z}_i'$$

Hence  $\mathbf{y}$  has pdf

$$f_y(\mathbf{y}) = (2\pi)^{-n/2} \exp \left\{ -\frac{1}{2} (\mathbf{y} - \mathbf{x}\beta)' \Sigma^{-1} (\mathbf{y} - \mathbf{x}\beta) \right\}$$

Taking logs gives the log-likelihood

$$\ell = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log|\Sigma| - \frac{1}{2} (\mathbf{y} - \mathbf{x}\beta)' \Sigma^{-1} (\mathbf{y} - \mathbf{x}\beta)$$

Differentiating w.r.t.  $\beta$  and  $\sigma_i^2$  leads to the ML equations

$$0 = \mathbf{x}' \Sigma^{-1} (\mathbf{y} - \mathbf{x}\beta) \quad \text{or} \quad \mathbf{x}' \Sigma^{-1} \mathbf{x}\beta = \mathbf{x}' \Sigma^{-1} \mathbf{y} \quad (1)$$

and

$$\begin{aligned} 0 &= \frac{\partial}{\partial \sigma_i^2} \log|\Sigma| + \frac{\partial}{\partial \sigma_i^2} (\mathbf{y} - \mathbf{x}\beta)' \Sigma^{-1} (\mathbf{y} - \mathbf{x}\beta) \\ &\quad i=0, 1, \dots, q \\ &= \frac{\partial}{\partial \sigma_i^2} \log|\Sigma| + (\mathbf{y} - \mathbf{x}\beta)' \frac{\partial}{\partial \sigma_i^2} \Sigma^{-1} (\mathbf{y} - \mathbf{x}\beta) \quad (2) \end{aligned}$$

Lemma #1 (Searle, Casella, McCulloch)

If  $A = A(t)$  is nonsingular, then

$$\frac{dA^{-1}}{dt} = -A^{-1} \frac{dA}{dt} A^{-1}$$

Proof:  $AA^{-1} = I$  implies

$$\frac{\partial A}{\partial t} A^{-1} + A \frac{\partial A^{-1}}{\partial t} = 0 \quad \blacksquare$$

Lemma #2

$$\frac{\partial}{\partial t} \log |A| = \text{tr} \left\{ A^{-1} \frac{\partial A}{\partial t} \right\}$$

Using the lemmas (2) becomes  $\sum_{i=1}^q$

$$\text{tr} \left\{ \Sigma^{-1} \frac{\partial \Sigma}{\partial \sigma_i^2} \right\} = (y - X\beta)' \Sigma^{-1} \frac{\partial \Sigma}{\partial \sigma_i^2} (y - X\beta)$$

and since  $\Sigma = \sum_{i=0}^q \sigma_i^2 Z_i Z_i'$

$$(2) \quad \text{tr} \left\{ \Sigma^{-1} Z_i Z_i' \right\} = (y - X\beta)' \Sigma^{-1} Z_i Z_i' \Sigma^{-1} (y - X\beta)$$

If  $X$  is full column rank then (1)  
has a unique solution

$$\hat{\beta} = (X' \Sigma^{-1} X)^{-1} X' \Sigma^{-1} y$$

Even if  $X$  is not full column rank, we  
will show later that  $\hat{\mu} = X\hat{\beta}$  is unique

where  $\hat{\beta} = (X' \Sigma^{-1} X)^{-1} X' \Sigma^{-1} y$

$[A^-$  is g-inverse of  $A$  if  $AA^-A = A]$

Note that

$$\begin{aligned}\Sigma^{-1} (y - \hat{x}\hat{\beta}) &= (\Sigma^{-1} - \Sigma^{-1}X(X'\Sigma^{-1}X)^{-1}X'\Sigma^{-1})y \\ &= P_y\end{aligned}$$

So substituting  $\hat{x}\hat{\beta}$  for  $x\beta$  in (2) gives

$$(2) \quad \text{tr}(\Sigma^{-1} Z_i Z_i') = y' P' Z_i Z_i P y$$

$i = 0, 1, \dots, q$