

Problem 5.12

a treatments, n replicates/treatment

$$\begin{array}{cccc} 1 & 2 & \dots & a \\ Y_{11} & & & Y_{a1} \\ Y_{12} & & & \vdots \\ \vdots & & & \\ Y_{1n} & & & Y_{an} \end{array}$$

$$Y = \beta_0 \mathbf{1}_a \otimes \mathbf{1}_n + (X^* \otimes \mathbf{1}_n) \beta + E$$

$$Y \sim N\left[\mu, \Sigma = I_a \otimes (\sigma_1^2 I_n + \sigma_2^2 J_n)\right]$$

$$X^* \text{ } a \times p \quad 1' X^* = 0 \quad p < a-1$$

$$A_1 = \bar{J}_a \otimes \bar{J}_n \quad \text{intercept}$$

$$A_1 \Sigma = (\sigma_1^2 + n \sigma_2^2) A_1$$

$$A_2 = X^* (X^{*'} X^*)^{-1} X^{*'} \otimes \bar{J}_n \quad \text{regression}$$

$$A_2 \Sigma = (\sigma_1^2 + n \sigma_2^2) A_2$$

$$A_4 = I_a \otimes G_n \quad \text{pure error}$$

$$A_4 \Sigma = \sigma_1^2 A_4$$

$$A_3 = I_a \otimes I_n - A_1 - A_2 - A_4 \quad \text{lack of fit}$$

$$A_3 = [G_a - X^* (X^{*'} X^*)^{-1} X^{*'}] \otimes \bar{J}_n$$

$$A_3 \Sigma = (\sigma_1^2 + n \sigma_2^2) A_3$$

$$\text{Then } \sum_{i=1}^4 A_i = I_a \otimes I_n$$

$$\sum = \sum_i c_i A_i \quad c_1 = c_2 = c_3 = (\sigma_1^2 + n\sigma_2^2) \\ c_4 = \sigma_1^2$$

$$Y' A_2 Y \sim \chi_p^2 (\lambda_2) (\sigma_1^2 + n\sigma_2^2)$$

$$\lambda_2 = Y' A_2 Y = \frac{n \beta' (X^* X^*)^{-1} \beta}{\sigma_1^2 + n\sigma_2^2}$$

$$Y' A_3 Y \sim \chi_{a-p-1}^2 (0) (\sigma_1^2 + n\sigma_2^2) \quad \text{if no lack of fit}$$

$$\lambda_3 = Y' A_3 Y$$

$$A_3 Y = [ (C_a - X^* (X^* X^*)^{-1} X^*) \otimes I_n ] \\ \times [ (I_a \otimes I_n) \beta_0 + (X^* \otimes I_n) \beta ] \\ = 0 + (X^* \otimes I_n) \beta - (X^* \otimes I_n) \beta = 0$$

$$\text{b/c } C_a I_a = 0 \quad X^* I_a = 0$$

F-statistic for testing  $H_0: \beta = 0$  is

$$\frac{Y' A_2 Y / p}{Y' A_3 Y / (a-p-1)} \sim F_{a, a-p-1} (\lambda_2) \\ \underbrace{\text{if no lack of fit}}$$

## The BLUP and Penalized Least Squares

### Penalized Spline Regression

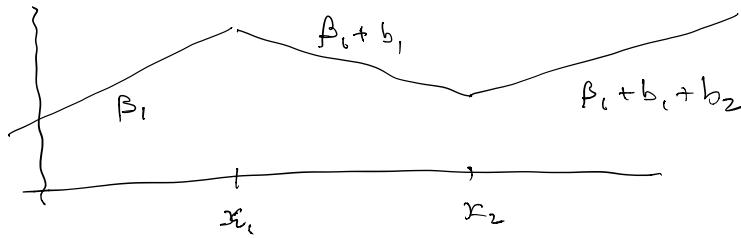
$$(x_i, y_i) \quad y_i = f(x_i) + e_i \quad i=1, \dots, n$$

#### Linear Spline Model

$$f(x) = \beta_0 + \beta_1 x + \sum_{j=1}^K b_j (x - x_j)_+$$

knots  $\min(x_i) < \kappa_1 < \dots < \kappa_K < \max(x_i)$

$$(x - x_j)_+ = \max(0, x - \kappa_j)$$



Fit by least squares with  $X = (1, x, (x - x_1)_+, \dots, (x - x_K)_+)^T$

### Penalized Least Squares

$$\text{minimize } \|y - X\beta\|^2 \text{ subject to } \beta^T A \beta \leq C$$

where  $A$  psd. and  $C > 0$ . Equivalent to

$$\text{minimize } \|y - X\beta\|^2 + \lambda \beta^T A \beta$$

for some  $\lambda$

Solution is  $\hat{\beta} = (X'X + \lambda A)^{-1} X'y$

### Penalized Splines as BLUPs

Consider the linear mixed model

$$y_i = \beta_0 + \beta_1 x_i + \sum_{j=1}^K u_j (x_i - x_j)_+ + \varepsilon_i \\ = X\beta + Z u + \varepsilon$$

$$u_j \sim N(0, \sigma_u^2) \quad \varepsilon_i \sim N(0, \sigma_\varepsilon^2)$$

The BLUP for  $f(x) = \beta_0 + \beta_1 x + \sum_{j=1}^K u_j (x - x_j)_+$   
is obtain by minimizing

$$\frac{1}{\sigma_\varepsilon^2} \|y - X\beta - Zu\|^2 + \frac{1}{\sigma_u^2} u'u$$

$$\text{or } \|y - X\beta - Zu\|^2 + \lambda u'u \text{ where } \lambda = \sigma_u^2 / \sigma_\varepsilon^2$$


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### EM Algorithm

$y$  observable data

$z$  missing / latent data

$\theta$  parameter

$$\ell_C = \log f(y, z; \theta) \quad \begin{matrix} \text{complete data} \\ \text{log likelihood} \end{matrix}$$

$$\ell = \log \int f(y, z; \theta) dz \quad \begin{matrix} \text{marginal log} \\ \text{likelihood} \end{matrix}$$

$Q$ -function - E-step

$$Q(\theta, \theta^*) = E_{\theta^*} \left\{ \log f(y, z; \theta) \mid y \right\}$$

M-step

$$\theta^{t+1} = \arg \max_{\theta} Q(\theta; \theta^*)$$


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Application to Variance Components Models

$$Y = X\beta + \sum_{i=0}^q Z_i u_i + E$$

$$L_c = -\frac{1}{2} \left( \sum_{i=0}^q c_i \right) \log 2\pi - \frac{1}{2} \sum_{i=0}^q c_i \log \sigma_i^2$$

$$- \frac{1}{2} \sum_{i=1}^q \frac{1}{\sigma_i^2} \|u_i\|^2 - \underbrace{\frac{1}{2\sigma_0^2} \|y - X\beta - \sum_{i=0}^q Z_i u_i\|^2}_{\|u_0\|^2}$$

Also

$$\|y - X\beta - \sum_i Z_i u_i\|^2 = \|y - \hat{X}\hat{\beta} - \sum_i Z_i u_i\|^2$$

$$+ \|X\beta - \hat{X}\hat{\beta}\|^2$$

where  $\hat{X}\hat{\beta} = X(X'X)^{-1}X' \left( y - \sum_i Z_i u_i \right)$   $= X\beta + u_0$

It follows that the EM update eqns are

$$\hat{X}\hat{\beta}^{(t+1)} = X(X'X)^{-1}X' \left[ \hat{X}\hat{\beta}^{(t)} + E^{(t)}(u_0 | y) \right]$$

$$\hat{\sigma}_i^{(t+1)} = \frac{1}{c_i} E^{(t)}( \|u_i\|^2 | y ) \quad i=0, 1, \dots, q$$

## Summary

Step 0 : Choose starting values  $\beta^{(0)}, \sigma_i^{2(0)} \ i=0, 1, \dots, q$

Step 1 : E-step

$$\text{Set } \hat{t}_i^{(t+1)} = E^{(t)}(u_i' u_i | y)$$

$$\text{and } \hat{s}^{(t+1)} = E^{(t)}(x \hat{\beta}^{(t)} + u_0 | y)$$

Step 2 : M-step

$$\hat{\sigma}_i^{2(t+1)} = \hat{t}_i^{(t+1)} / c_i \quad i=0, 1, \dots, q$$

$$x \hat{\beta}^{(t+1)} = x' x^{-1} x' \hat{s}^{(t)}$$