

Talk on 2010-07-09: The EM-REML algorithm(3)

The simple model:

$$Y = X\gamma + H\beta + e$$

where

$$Y : N \times 1,$$

$$X : N \times p,$$

$$\gamma : p \times 1, \gamma \text{ is the fixed effect},$$

$$H : N \times q,$$

$$\beta : q \times 1, \beta \sim MN(0, \tau R),$$

and $e : N \times 1, e \sim MN(0, \sigma I)$.

Let $U = A^T Y$ with the condition that $A^T A = I_{N-p}$ and $AA^T = I - P_X = I - X(X^T X)^{-1}X^T$, we have

$$\begin{aligned} E(U) &= E(A^T Y) \\ &= E(A^T X\gamma + A^T H\beta + A^T e) \\ &= A^T X\gamma \end{aligned}$$

Consider that,

$$\begin{aligned} (A^T X\gamma)^T (A^T X\gamma) &= \gamma^T X^T AA^T X\gamma \\ &= \gamma^T X^T \underbrace{(I - P_X)}_0 X\gamma \\ &= 0 \end{aligned}$$

Therefore $A^T X\gamma = 0$, so $E(U) = 0$.

Define $\text{Var}(Y) = V = \tau H R H^T + \sigma I$, so we have $\text{Var}(U) = A^T V A$.

Since U and β are normal distributed, the joint distribution of them is also normal distributed, the covariance of U and β is

$$\begin{aligned} \text{Cov}(U, \beta) &= \text{Cov}(A^T X\gamma + A^T H\beta + A^T e, \beta) \\ &= \text{Cov}(A^T H\beta, \beta) \\ &= A^T H \text{Var}(\beta) = \tau A^T H R \end{aligned}$$

Therefore, the joint distribution of $(U, \beta)^T$ is

$$\begin{pmatrix} U \\ \beta \end{pmatrix} \sim MN\left(\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \Sigma = \begin{pmatrix} A^T V A & \tau A^T H R \\ \tau R H^T A & \tau R \end{pmatrix}\right)$$

According to $E(\mu_1|\mu_2) = \mu_1 + \Sigma_{12}(\Sigma_{22})^{-1}\mu_2$ and $Var(\mu_1|\mu_2) = \Sigma_{11}(\Sigma_{22})^{-1}\Sigma_{21}$.

$$\begin{aligned} E(U|\beta) &= 0 + \tau A^T H R \tau^{-1} R^{-1} \beta \\ &= A^T H \beta \\ Var(U|\beta) &= A^T V A - \tau A^T H R \tau^{-1} R^{-1} \tau R H^T A \\ &= A^T V A - A^T (\tau H R H^T) A \\ &= A^T (V - \tau H R H^T) A \\ &= A^T \cdot \sigma I \cdot A \\ &= \sigma I \end{aligned}$$

Therefore, we have the conditional distribution of $U|\beta$ which is

$$U|\beta \sim MN(A^T H \beta, \sigma I_{N-p})$$

For $\beta|U$, we have

$$\begin{aligned} E(\beta|U) &= 0 + \tau R H^T A \cdot (A^T V A)^{-1} \cdot A^T Y \\ &= \tau R H^T \cdot A (A^T V A)^{-1} A^T \cdot Y \\ Var(\beta|U) &= \tau R - \tau R H^T A \cdot (A^T V A)^{-1} \cdot \tau A^T H R \\ &= \tau R - \tau^2 R H^T \cdot A (A^T V A)^{-1} A^T \cdot \tau H R \end{aligned}$$

To show that $A(A^T V A)^{-1} A^T = P = V^{-1} - V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1}$, we constructing the $n \times p$ matrix $\mathbf{G} = \mathbf{V}^{-1} \mathbf{X} (\mathbf{X}^T \mathbf{V}^{-1} \mathbf{X})^{-1}$ and the $n \times n$ matrix $\mathbf{B} = [\mathbf{A} | \mathbf{G}]$. First the product,

$$\mathbf{B}^T \mathbf{B} = \begin{bmatrix} \mathbf{A}^T \\ \mathbf{G}^T \end{bmatrix} [\mathbf{A} \quad \mathbf{G}] = \begin{bmatrix} \mathbf{A}^T \mathbf{A} & \mathbf{A}^T \mathbf{G} \\ \mathbf{G}^T \mathbf{A} & \mathbf{G}^T \mathbf{G} \end{bmatrix}$$

then the determinant can be rewritten as

$$\begin{aligned} |\mathbf{B}|^2 &= |\mathbf{B}' \mathbf{B}| = |\mathbf{A}' \mathbf{A}| \times |\mathbf{G}' \mathbf{G} - \mathbf{G}' \mathbf{A} (\mathbf{A}' \mathbf{A})^{-1} \mathbf{A}' \mathbf{G}| \\ &= |\mathbf{I}| \times |\mathbf{G}' \mathbf{G} - \mathbf{G}' (\mathbf{I} - \mathbf{P}_X) \mathbf{G}| = |\mathbf{G}' \mathbf{P}_X \mathbf{G}| \\ &= |(\mathbf{X}' \mathbf{V}^{-1} \mathbf{X})^{-1} \mathbf{X}' \mathbf{V}^{-1} \mathbf{X} (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}' \mathbf{V}^{-1} \mathbf{X} (\mathbf{X}' \mathbf{V}^{-1} \mathbf{X})^{-1}| = |(\mathbf{X}' \mathbf{X})^{-1}|. \end{aligned}$$

$$\begin{aligned}
(A^T V G)^T (A^T V G) &= G^T V A A^T V G \\
&= G^T V \underbrace{(I - P_X) V V^{-1} X (X^T V^{-1} X)^{-1}}_0 \\
&= 0
\end{aligned}$$

which also says that \mathbf{B} is nonsingular.

$$\begin{aligned}
V^{-1} &= B(B^T V B)^{-1} B^T \\
&= [A \quad G] \begin{bmatrix} A^T V A & 0 \\ 0 & G^T V G \end{bmatrix} \begin{bmatrix} A^T \\ G^T \end{bmatrix} \\
&= A(A^T V A)^{-1} A^T + G(G^T V G)^{-1} G^T \\
&= A(A^T V A)^{-1} A^T + G \underbrace{((X^T V^{-1} X)^{-1} X^T V^{-1} V V^{-1} X (X^T V^{-1} X)^{-1})^{-1}}_{X^T V^{-1} X} G^T \\
&= A(A^T V A)^{-1} A^T + V^{-1} X (X^T V^{-1} X)^{-1} \cdot X^T V^{-1} X \cdot (X^T V^{-1} X)^{-1} X^T V^{-1} \\
&= A(A^T V A)^{-1} A^T + V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1}
\end{aligned}$$

so we have $A(A^T V A)^{-1} A^T = P = V^{-1} - V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1}$. Therefore, the expectation and variance of $\beta|U$ can be simplified as

$$\begin{aligned}
E(\beta|U) &= \tau R H^T P_X Y \\
Var(\beta|U) &= \tau R - \tau^2 R H^T P_X H R
\end{aligned}$$

In another words, we have,

$$\beta|U \sim MN(\tau R H^T P_X Y, \tau R - \tau^2 R H^T P_X H R)$$

Define $\theta = \{\sigma, \tau\}$, according to the EM algorithm, we need to first compute the expectation of $\log L(\theta^{(t)}|U, \beta)$ given U and $\theta^{(t-1)}$,

$$\begin{aligned}
\log L(\theta^{(t)}|U, \beta) &= \log f(U, \beta|\theta^{(t)}) \\
&= \log\{f(U|\beta, \theta^{(t)})f(\beta|\theta^{(t)})\} \\
&= \log f(U|\beta, \theta^{(t)}) + \log f(\beta|\theta^{(t)})
\end{aligned}$$

1. Estimate τ Take the expectation of $\log L(\theta^{(t)}|U, \beta)$ with $\beta|U, \theta^{(t-1)}$, we have

$$E_\beta \left[\log L(\theta^{(t)}|U, \beta) \middle| U, \theta^{(t-1)} \right] = E_\beta \left[\log f(U|\beta, \theta^{(t)}) \middle| U, \theta^{(t-1)} \right] - \frac{1}{2} q \log \tau - \frac{1}{2} \log |R| - \frac{1}{2\tau} E_\beta \left[(\beta^T R^{-1} \beta) \middle| U, \theta^{(t-1)} \right]$$

Since the $E(\varepsilon^T \Lambda \varepsilon) = E(\varepsilon)^T \Lambda E(\varepsilon) + \text{tr}(\Lambda \text{Var}(\varepsilon))$, (1) can be simplified as

$$\begin{aligned} E_{\beta|U, \theta^{(t-1)}}(\log L(\theta^{(t)}|U, \beta)) = & E_{\beta} \left[\log f(U|\beta, \theta^{(t)}) \middle| U, \theta^{(t-1)} \right] - \frac{1}{2} q \log \tau - \frac{1}{2} \log |R| \\ & - \frac{1}{2\tau} \left[E(\beta|U, \theta^{(t-1)})^T R^{-1} E(\beta|U, \theta^{(t-1)}) + \text{tr}(R^{-1} \text{Var}(\beta|U, \theta^{(t-1)})) \right] \end{aligned}$$

To maximize the expectation above, we let

$$\frac{\partial E_{\beta|U, \theta^{(t-1)}}(\log L(\theta^{(t)}|U, \beta))}{\partial \theta} = 0$$

It is easily to derive that

$$\tau^{(t)} = \frac{1}{q} \left[E(\beta|U, \theta^{(t-1)})^T R^{-1} E(\beta|U, \theta^{(t-1)}) + \text{tr}(R^{-1} \text{Var}(\beta|U, \theta^{(t-1)})) \right] \quad (1)$$

2. Estimate σ We can also get the estimation of σ by Define

$$\begin{aligned} Q = & E_{\beta} \left[(\log L(\theta^{(t)}|U, \beta)) \middle| U, \theta^{(t-1)} \right] \\ = & E_{\beta} \left[-\frac{1}{2} \left[(N-p) \log \sigma + 1 + \frac{1}{\sigma} (U - A^T H \beta)^T (U - A^T H \beta) \right] \middle| U, \theta^{(t-1)} \right] \\ & + E_{\beta} \left[\log f(\beta|\theta^{(t)}) \middle| U, \theta^{(t-1)} \right] \end{aligned}$$

If we take the expectation on β , then

$$\begin{aligned} & E_{\beta}[\log(L)|U, \theta^{(t-1)}] \\ = & E_{\beta} \left[-\frac{1}{2} (N-p) \log \sigma + 1 + \frac{1}{\sigma} \left((Y - H\beta)^T A A^T (Y - H\beta) \right) + \log f(\beta|\theta^{(t)}) \middle| U, \theta^{(t-1)} \right] \\ = & -\frac{1}{2} (N-p) \log \sigma + 1 + \frac{1}{\sigma} \left((Y - H\tilde{\beta})^T (I - P_X) (Y - H\tilde{\beta}) + \text{tr}(H^T (I - P_X) H \text{Var}(\beta|U)) \right) \\ & + E_{\beta} \left[\log f(\beta|\theta^{(t)}) \middle| U, \theta^{(t-1)} \right] + 1 \end{aligned}$$

Let $\frac{\partial Q}{\partial \sigma} = 0$, we have

$$\sigma^{(t)} = \frac{1}{N-p} \left[(Y - H\tilde{\beta})^T (I - P_X) (Y - H\tilde{\beta}) + \text{tr}(H^T (I - P_X) H \text{Var}(\beta|U)) \right] \quad (2)$$

If the model is

$$Y = X\gamma + H_A \beta_A + H_B \beta_B + e$$

where

$$Y : N \times 1,$$

$$X : N \times p,$$

$\gamma : p \times 1$, γ is the fixed effect,

$$H_A : N \times q_A,$$

$$\beta_A : q_A \times 1, \beta \sim MN(0, \tau_A R_A),$$

$$H_B : N \times q_B,$$

$$\beta_B : q_B \times 1, \beta \sim MN(0, \tau_B R_B),$$

construct $H = [H_A H_B]$, $\beta = (\beta_A, \beta_B)^T$ and $R = \begin{bmatrix} \tau_A R_A & 0 \\ 0 & \tau_B R_B \end{bmatrix}$. According to the simple model, we can easily get that

$$\begin{pmatrix} U \\ \beta \end{pmatrix} \sim MN\left(\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \Sigma = \begin{pmatrix} A^T V A & A^T H R \\ R H^T A & \tau R \end{pmatrix}\right)$$

and

$$E(U|\beta) = A^T H \beta$$

$$Var(U|\beta) = \sigma I_{N-p}$$

$$E(\beta|U) = R H^T P Y$$

$$Var(\beta|U) = R - R H^T P H R$$

The likelihood function is

$$\begin{aligned} \log L(\theta^{(t)}|U, \beta) &= \log f(U, \beta|\theta^{(t)}) \\ &= \log f(U|\beta, \theta^{(t)}) + \log f(\beta|\theta^{(t)}) \\ &= \left(-\frac{1}{2}\right) \left[\log \left| \begin{bmatrix} \tau_A R_A & 0 \\ 0 & \tau_B R_B \end{bmatrix} \right| + (\beta_A \quad \beta_B)^T \begin{bmatrix} (\tau_A R_A)^{-1} & 0 \\ 0 & (\tau_B R_B)^{-1} \end{bmatrix} \begin{bmatrix} \beta_A \\ \beta_B \end{bmatrix} \right] \\ &\quad + \log f(U|\beta, \theta^{(t)}) \\ &= \log f(U|\beta, \theta^{(t)}) + \log f(\beta_A|\theta^{(t)}) + \log f(\beta_B|\theta^{(t)}) \end{aligned}$$

so the estimation of θ is

$$\tau_A^{(t)} = \frac{1}{q_A} \left[E(\beta_A|U, \theta^{(t-1)})^T R_A^{-1} E(\beta_A|U, \theta^{(t-1)}) + tr(R_A^{-1} Var(\beta_A|U, \theta^{(t-1)})) \right] \quad (3)$$

$$\tau_B^{(t)} = \frac{1}{q_B} \left[E(\beta_B|U, \theta^{(t-1)})^T R_B^{-1} E(\beta_B|U, \theta^{(t-1)}) + tr(R_B^{-1} Var(\beta_B|U, \theta^{(t-1)})) \right] \quad (4)$$

$$\sigma^{(t)} = \frac{1}{N-p} \left[(Y - H\tilde{\beta})^T (I - P_X) (Y - H\tilde{\beta}) + tr(H^T (I - P_X) H Var(\beta|U)) \right] \quad (5)$$

APPENDIX

The variables we used in the algorithm are

$$P_X = X(X^T X)^{-1} X^T$$

$$V = \tau H R H^T + \sigma I$$

$$P = V^{-1} - V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1}$$

$$E(\beta|U) = \tau R H^T P Y$$

$$Var(\beta|U) = \tau R - \tau^2 R H^T P H R$$

$$\tau^{(t)} = \frac{1}{q} \left[E(\beta|U, \theta^{(t-1)})^T R^{-1} E(\beta|U, \theta^{(t-1)}) + tr(R^{-1} Var(\beta|U, \theta^{(t-1)})) \right]$$

$$\sigma^{(t)} = \frac{1}{N-p} \left[(Y - H\tilde{\beta})^T (I - P_X) (Y - H\tilde{\beta}) + tr(H^T (I - P_X) H Var(\beta|U)) \right]$$

Also, we have a algorithm for computing the inverse of a special form of matrix

$$(I + BC)^{-1} = I - B(I + CB)^{-1}C$$

So if we have to big matrix in the form of $(I + A)$ where A is $m \times m$, we can try to split A into $A = BC$ where B is $m \times n$ and n is much smaller than m.