Integrating over the random effects in a Bayesian hierarchical model

(first draft) by Jesse

I. Some lemmas

Completing the square in matrix form

If **A** is symmetric and invertible,

$$y'Ay - 2b'y = (y - A^{-1}b)'A(y - A^{-1}b) - b'A^{-1}b$$
, or equivalently,

$$y'Ay - 2b'y + b'A^{-1}b = (y - A^{-1}b)'A(y - A^{-1}b).$$

Proof

Starting with the right hand side,

$$(y - A^{-1}b)'A(y - A^{-1}b) - b'A^{-1}b$$

= $y'Ay - y'AA^{-1}b - b'(A^{-1})'Ay + b'(A^{-1})'AA^{-1}b - b'A^{-1}b$

and simplifying and using the symmetry of A, we have

$$= \mathbf{y}' \mathbf{A} \mathbf{y} - 2 \mathbf{b}' \mathbf{y}. \blacksquare$$

Proposition

If random vector \mathbf{y} has density $f(\mathbf{y}) \propto \exp\left\{-\frac{1}{2}Q(\mathbf{y})\right\}$, where $Q(\mathbf{y}) = (\mathbf{y} - \mathbf{m})'V^{-1}(\mathbf{y} - \mathbf{m})$,

then $y \sim N_k(\boldsymbol{m}, \boldsymbol{V})$.

<u>Proof</u>

Suppose $f(y) = C \exp\left\{-\frac{1}{2}Q(y)\right\}$ for some constant $C \neq 0$.

Then
$$f(\mathbf{y}) = C \left[(2\pi)^{-\frac{k}{2}} |\mathbf{V}|^{-\frac{1}{2}} \right]^{-1} (2\pi)^{-\frac{k}{2}} |V|^{-\frac{1}{2}} \exp\left\{ -\frac{1}{2} Q(\mathbf{y}) \right\}.$$

The quantity $(2\pi)^{-\frac{k}{2}}|V|^{-\frac{1}{2}}\exp\left\{-\frac{1}{2}Q(y)\right\}$ is a multivariate normal density,

so integrating both sides wrt \mathbf{y} gives $1 = C \left[(2\pi)^{-\frac{k}{2}} |\mathbf{V}|^{-\frac{1}{2}} \right]^{-1}$,

so
$$C = (2\pi)^{-\frac{k}{2}} |V|^{-\frac{1}{2}}$$
, so $f(y) = (2\pi)^{-\frac{k}{2}} |V|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}Q(y)\right\}$,

which is the $N_k(\boldsymbol{m}, \boldsymbol{V})$ density.

Proposition

If
$$f(y) \propto \exp\left\{-\frac{1}{2}Q(y)\right\}$$
,
where $Q(y) = y'V^{-1}y - 2m'V^{-1}y$,
then $y \sim N_k(m, V)$.

Proof

Rewrite
$$Q(y)$$
 as $(y-m)'V^{-1}(y-m) - m'V^{-1}m$, so that we have
$$f(y) \propto \exp\left\{-\frac{1}{2}(y-m)'V^{-1}(y-m)\right\} \exp\left\{-\frac{1}{2}m'V^{-1}m\right\}$$
$$\propto \exp\left\{-\frac{1}{2}(y-m)'V^{-1}(y-m)\right\},$$

and the conclusion follows by the previous result. ■

Proposition

If
$$f(\mathbf{y}) \propto \exp\left\{-\frac{1}{2}Q(\mathbf{y})\right\}$$
,
where $Q(\mathbf{y}) = \mathbf{y}'A\mathbf{y} - 2\mathbf{b}'\mathbf{y}$, and \mathbf{A} is pd,
then $\mathbf{y} \sim N_k(\mathbf{A}^{-1}\mathbf{b}, \mathbf{A}^{-1})$.

Proof

Suppose
$$Q(y) = y'Ay - 2b'y$$
, and also $Q(y) = y'V^{-1}y - 2m'V^{-1}y$ for some m, V .
Then $A = V^{-1}$, so $V = A^{-1}$.
Also $b' = m'V^{-1}$, so $b = V^{-1}m$, so $m = Vb = A^{-1}b$.
Therefore by the previous proposition, $y \sim N_k(A^{-1}b, A^{-1})$.

II. Model specification in matrix form

For y_{ijk} and ϵ_{ijk} , i is subject, j is timepoint, k is outcome.

In this model we have *J* timepoints and 3 outcomes.

For x_{ip} , α_{ip} , and β_{ip} , i is subject, p is index.

Ignore the effect of diagnostic group for now.

The matrix equation for subject i is $y_i = X_i \alpha_i + W_i \beta_i + \epsilon_i$, or

with $\epsilon_i \sim N_{3I}(0, V)$, and with $V = I_I \otimes \Sigma$,

where Σ is the (3 × 3) covariance matrix of the outcomes, and with $\beta_i \sim N_6(\mu, \Omega)$.

For compactness, we might write

$$X_{i} = \mathbf{1}_{J} \otimes I_{3} \otimes x'_{i}$$

$$W_{i} = \begin{bmatrix} I_{3} \otimes \begin{bmatrix} 1 & t_{i1} \end{bmatrix} \\ \dots \\ I_{3} \otimes \begin{bmatrix} 1 & t_{iJ} \end{bmatrix} \end{bmatrix}.$$

III. Integrating out β

Assume X, α , W, Σ , μ , Ω are known. To integrate out β , use the relationship $f(y) = \int f(y|\beta)f(\beta)d\beta$.

The densities are

$$f(y|\beta) \propto \exp\left\{-\frac{1}{2}Q_1(y,\beta)\right\}$$
 and $f(\beta) \propto \exp\left\{-\frac{1}{2}Q_2(\beta)\right\}$,

where (dropping subscripts)

$$Q_1(y, \boldsymbol{\beta}) = (y - X\alpha - W\beta)'V^{-1}(y - X\alpha - W\beta)$$
$$Q_2(\boldsymbol{\beta}) = (\boldsymbol{\beta} - \boldsymbol{\mu})'\Omega^{-1}(\boldsymbol{\beta} - \boldsymbol{\mu})$$

so the joint density is

$$\propto \exp\left\{-\frac{1}{2}Q(\mathbf{y},\boldsymbol{\beta})\right\}$$

where $Q(y, \beta) = Q_1(y, \beta) + Q_2(\beta)$.

We add the quadratic forms and refactor as follows:

$$\begin{split} Q_{1}(y,\beta) + Q_{2}(\beta) &= (y - X\alpha - W\beta)'V^{-1}(y - X\alpha - W\beta) + (\beta - \mu)'\Omega^{-1}(\beta - \mu) \\ &= y'V^{-1}y - y'V^{-1}X\alpha - y'V^{-1}W\beta - \alpha'X'V^{-1}y + \alpha'X'V^{-1}X\alpha + \alpha'X'V^{-1}W\beta \\ &- \beta'W'V^{-1}y + \beta'W'V^{-1}X\alpha + \beta'W'V^{-1}W\beta + \beta'\Omega^{-1}\beta - 2\mu'\Omega^{-1}\beta + \mu'\Omega^{-1}\mu \\ &= y'[V^{-1}]y - 2[\alpha'X'V^{-1}]y \\ &- 2\beta'[W'V^{-1}]y \\ &+ \beta'[W'V^{-1}W + \Omega^{-1}]\beta - 2[\mu'\Omega^{-1} - \alpha'X'V^{-1}W]\beta \\ &+ \alpha'X'V^{-1}X\alpha + \mu'\Omega^{-1}\mu \\ &= \beta'[W'V^{-1}W + \Omega^{-1}]\beta - 2[y'V^{-1}W + \mu'\Omega^{-1} - \alpha'X'V^{-1}W]\beta \\ &+ y'[V^{-1}]y - 2[\alpha'X'V^{-1}]y + \alpha'X'V^{-1}X\alpha + \mu'\Omega^{-1}\mu. \end{split}$$

Let $A = W'V^{-1}W + \Omega^{-1}$, and let $b' = y'V^{-1}W + \mu'\Omega^{-1} - \alpha'X'V^{-1}W$, noting that b depends on y, and we have

$$\begin{aligned} Q_{1}(y,\beta) + Q_{2}(\beta) \\ &= \beta' A \beta - 2b' \beta + b' A^{-1} b \\ &+ y' [V^{-1}] y - 2[\alpha' X' V^{-1}] y + \alpha' X' V^{-1} X \alpha + \mu' \Omega^{-1} \mu - b' A^{-1} b \\ &= (\beta - A'b)' A (\beta - A^{-1}b) \\ &+ y' [V^{-1}] y - 2[\alpha' X' V^{-1}] y + \alpha' X' V^{-1} X \alpha + \mu' \Omega^{-1} \mu - b' A^{-1} b. \end{aligned}$$

Now if we integrate over β , the kernel

$$\propto \exp\left\{-\frac{1}{2}(\boldsymbol{\beta} - \boldsymbol{A^{-1}}'\boldsymbol{b})'\boldsymbol{A}(\boldsymbol{\beta} - \boldsymbol{A^{-1}}\boldsymbol{b})\right\}$$

becomes 1, and we have

$$Q(y) = y'[V^{-1}]y - 2[\alpha'X'V^{-1}]y + \alpha'X'V^{-1}X\alpha + \mu'\Omega^{-1}\mu - b'A^{-1}b.$$

At this point, WLOG we let $X\alpha = 0$, remembering to add it to the mean of y at the end:

$$b' = y'V^{-1}W + \mu'\Omega^{-1}$$

$$Q(y) = y'[V^{-1}]y + \mu'\Omega^{-1}\mu - (y'V^{-1}W + \mu'\Omega^{-1})A^{-1}(W'V^{-1}y + \Omega^{-1}\mu)$$

$$= y'[V^{-1}]y + \mu'\Omega^{-1}\mu - y'V^{-1}WA^{-1}W'V^{-1}y - 2\mu'\Omega^{-1}A^{-1}W'V^{-1}y + \mu'\Omega^{-1}A^{-1}\Omega^{-1}\mu = y'[V^{-1} + V^{-1}W(W'V^{-1}W + \Omega^{-1})^{-1}W'V^{-1}]y - 2[\mu'\Omega^{-1}(W'V^{-1}W + \Omega^{-1})^{-1}W'V^{-1}]y + \mu'[\Omega^{-1} + \Omega^{-1}(W'V^{-1}W + \Omega^{-1})^{-1}\Omega^{-1}]\mu.$$

Let $C = V^{-1} + V^{-1}W(W'V^{-1}W + \Omega^{-1})^{-1}W'V^{-1}$, and let $d' = \mu'\Omega^{-1}(W'V^{-1}W + \Omega^{-1})^{-1}W'V^{-1}$. Then we have $Q(y) = (y - C^{-1}d)'C(y - C^{-1}d) + [\text{other terms}]$, and so $y \sim N(C^{-1}d, C^{-1})$.

Adding back $X\alpha$, we finally have

$$y \sim N_{3J}(X\alpha + C^{-1}d, C^{-1})$$

$$C = V^{-1} + V^{-1}W(W'V^{-1}W + \Omega^{-1})^{-1}W'V^{-1}$$

$$d = V^{-1}W(W'V^{-1}W + \Omega^{-1})^{-1}\Omega^{-1}\mu.$$

Quick sanity check: do we see a β anywhere? No.

Another one: do dimensions match?

$$X$$
 is $(3J \times 6)$, α is (6×1) , so $X\alpha$ is $(3J \times 1)$
 V^{-1} is $(3J \times 3J)$, W is $(3J \times 6)$, so C and C^{-1} are $(3J \times 3J)$
 d is $(3J \times 1)$, so $C^{-1}d$ is $(3J \times 1)$
so they do match.

IV. Another method

This time we make the means of the random intercept and slope fixed, part of α , so that each β_i has mean 0.

The matrix equation for subject i is $y_i = X_i \alpha_i + W_i \beta_i + \epsilon_i$, or

$$+\begin{bmatrix} 1 & t_{i1} & & & & & \\ & & 1 & t_{i1} & & & \\ & & & 1 & t_{i1} & & \\ & & & & 1 & t_{i1} \\ & & & & & \ddots & \ddots & \\ 1 & t_{ij} & & & & & \\ & & & & 1 & t_{ij} & & \\ & & & & & 1 & t_{ij} \end{bmatrix} \begin{bmatrix} \beta_{i1} \\ \beta_{i2} \\ \beta_{i3} \\ \beta_{i4} \\ \beta_{i5} \\ \beta_{i6} \end{bmatrix} + \begin{bmatrix} \epsilon_{i11} \\ \epsilon_{i12} \\ \epsilon_{i13} \\ \vdots \\ \epsilon_{ij1} \\ \epsilon_{ij2} \\ \epsilon_{ij3} \end{bmatrix},$$

with $\epsilon_i \sim N_{3J}(\mathbf{0}, \mathbf{V})$, and with $\mathbf{V} = \mathbf{I}_J \otimes \mathbf{\Sigma}$,

where Σ is the (3 × 3) covariance matrix of the outcomes, and with $\beta_i \sim N_6(0, \Omega)$.

Assume X, α , W, Σ , Ω are known. To integrate out β , use the relationship $f(y) = \int f(y|\beta)f(\beta)d\beta$.

The densities are

$$f(\mathbf{y}|\boldsymbol{\beta}) \propto \exp\left\{-\frac{1}{2}Q_1(\mathbf{y},\boldsymbol{\beta})\right\}$$
 and $f(\boldsymbol{\beta}) \propto \exp\left\{-\frac{1}{2}Q_2(\boldsymbol{\beta})\right\}$,

where, dropping subscripts and letting $u = y - X\alpha$, we have

$$Q_1(u, \boldsymbol{\beta}) = (u - W\boldsymbol{\beta})'V^{-1}(u - W\boldsymbol{\beta})$$

$$Q_2(\boldsymbol{\beta}) = \boldsymbol{\beta}' \boldsymbol{\Omega}^{-1} \boldsymbol{\beta}$$

so the joint density is

$$\propto \exp\left\{-\frac{1}{2}Q(\boldsymbol{u},\boldsymbol{\beta})\right\}$$

where $Q(\mathbf{u}, \boldsymbol{\beta}) = Q_1(\mathbf{u}, \boldsymbol{\beta}) + Q_2(\boldsymbol{\beta})$.

$$\begin{aligned} Q_1(\pmb{u},\pmb{\beta}) + Q_2(\pmb{\beta}) &= (\pmb{u} - \pmb{W}\pmb{\beta})'\pmb{V}^{-1}(\pmb{u} - \pmb{W}\pmb{\beta}) + \pmb{\beta}'\pmb{\Omega}^{-1}\pmb{\beta} \\ &= u'V^{-1}u - 2u'V^{-1}W\beta + \beta'W'V^{-1}W\beta + \beta'\Omega^{-1}\beta \\ &= \beta'[\Omega^{-1} + W'V^{-1}W]\beta - 2[u'V^{-1}W]\beta + u'V^{-1}u \\ \text{Letting } A &= \Omega^{-1} + W'V^{-1}W \text{ and } b' = u'V^{-1}W, \text{ we have} \end{aligned}$$

$$= (\beta - A^{-1}b)'A(\beta - A^{-1}b) - b'A^{-1}b + u'V^{-1}u.$$

Now if we integrate over β , the kernel

$$\propto \exp\left\{-\frac{1}{2}(\boldsymbol{\beta} - \boldsymbol{A}^{-1}\boldsymbol{b})'\boldsymbol{A}(\boldsymbol{\beta} - \boldsymbol{A}^{-1}\boldsymbol{b})\right\}$$

becomes 1, and we have

$$Q(\mathbf{u}) = \mathbf{u}'V^{-1}\mathbf{u} - \mathbf{b}'A^{-1}\mathbf{b}$$

$$= u'V^{-1}u - u'V^{-1}W(\Omega^{-1} + W'V^{-1}W)^{-1}W'V^{-1}u$$

$$= u'[V^{-1} - V^{-1}W(\Omega^{-1} + W'V^{-1}W)^{-1}W'V^{-1}]u$$

which means that $u \sim N(0, C^{-1})$,

and so
$$y \sim N(X\alpha, C^{-1})$$
,

where
$$C = V^{-1} - V^{-1}W(\Omega^{-1} + W'V^{-1}W)^{-1}W'V^{-1}$$
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