Whiteboard Lecture

Laplace's Method and PQL

Whiteboard Interlude II

The likelihood is:

$$\mathcal{L}(\beta, \mathbf{G}, \phi) = (2\pi)^{-q/2} e^{-\mathbf{1}^T c(\mathbf{y})} |\mathbf{G}|^{-1/2} J \quad (\mathbf{u} \text{ is } q \times 1)$$

where

$$J = \int_{\mathbb{R}^q} e^{h(\mathbf{u})}\, d\mathbf{u}$$

and

$$h(\mathbf{u}) = \frac{\mathbf{y}^T(\mathbf{X}\beta + \mathbf{Zu}) - \mathbf{1}^T b(\mathbf{X}\beta + \mathbf{Zu})}{\phi} - \tfrac{1}{2}\mathbf{u}^T\mathbf{G}^{-1}\mathbf{u}.$$

Hence

$$\begin{aligned} dh(\mathbf{u}) &= \frac{\mathbf{y}^T\mathbf{Z}\, d\mathbf{u} - \mathbf{1}^T \text{diag}\{b'(\mathbf{X}\beta + \mathbf{Zu})\}\mathbf{Z}d\mathbf{u}}{\phi} - \mathbf{u}^T\mathbf{G}^{-1} d\mathbf{u} \\ &= \frac{1}{\phi}\{\mathbf{y} - b'(\mathbf{X}\beta + \mathbf{Zu})\}^T\mathbf{Z}\, d\mathbf{u} - \mathbf{u}^T\mathbf{G}^{-1} d\mathbf{u} \end{aligned}$$

By the First Identification Theorem

$$\mathsf{D}\, h(\mathbf{u}) = \frac{1}{\phi}\{\mathbf{y} - b'(\mathbf{X}\beta + \mathbf{Zu})\}^T\mathbf{Z} - \mathbf{u}^T\mathbf{G}^{-1}.$$

The stationary point $\mathbf{u}_0$ needed for Laplace's Method solves:

$$\mathsf{D}\, h(\mathbf{u}_0) = \mathbf{0}.$$

This can't be found analytically so need Newton-Raphson iteration:

$$\mathbf{u}_{0,i+1} = \mathbf{u}_{0,i} - \{\mathsf{H}h(\mathbf{u}_{0,i})\}^{-1}\mathsf{D}h(\mathbf{u}_{0,i})^T$$

The Hessian matrix required for this iteration can be shown to be

$$\mathrm{H}h(\mathbf{u}) = -\frac{1}{\phi}\mathbf{Z}^T\text{diag}\{b''(\mathbf{X}\beta + \mathbf{Z}\mathbf{u})\}\mathbf{Z} - \mathbf{G}^{-1}.$$

After obtaining $\mathbf{u}_0$ we approximate J by

$$e^{h(\mathbf{u}_0)}\sqrt{\frac{(2\pi)^q}{-|\mathrm{H}h(\mathbf{u}_0)|}}.$$

This leads to the approximate log-likelihood

$$\begin{aligned}\ell(\beta, \mathbf{G}, \phi) \;\simeq\; & \frac{\mathbf{y}^T(\mathbf{X}\beta + \mathbf{Z}\mathbf{u}_0) - \mathbf{1}^T b(\mathbf{X}\beta + \mathbf{Z}\mathbf{u}_0)}{\phi} \\ & +\mathbf{1}^T c(\mathbf{y}) - \tfrac{1}{2}\mathbf{u}_0^T\mathbf{G}^{-1}\mathbf{u}_0 \\ & -\tfrac{1}{2}\ln|\mathbf{I} + \mathbf{G}\mathbf{Z}^T\text{diag}\{b''(\mathbf{X}\beta + \mathbf{Z}\mathbf{u}_0)\}\mathbf{Z}|\end{aligned}$$

The last term is usually dropped, based on the argument that $b''(\mathbf{X}\beta + \mathbf{Z}\mathbf{u}_0)$ is relatively constant as a function of β, leading to:

$$\begin{aligned}\ell(\beta, \mathbf{G}, \phi) \;\simeq\; & \frac{\mathbf{y}^T(\mathbf{X}\beta + \mathbf{Z}\mathbf{u}_0) - \mathbf{1}^T b(\mathbf{X}\beta + \mathbf{Z}\mathbf{u}_0)}{\phi} \\ & +\mathbf{1}^T c(\mathbf{y}) - \tfrac{1}{2}\mathbf{u}_0^T\mathbf{G}^{-1}\mathbf{u}_0\end{aligned}$$

The GLMM approximate fitting method known as PQL involves estimation of β by maximisation of the right-hand side of above expression using Newton-Raphson iteration.

$\mathbf{G}$ and ϕ are estimated with other restricted log-likelihood approximations.

The main reference for this methodology is: Breslow, N.E. & Clayton, D.G. *J. American Statist. Assoc.*, 1993.

Question Why the name PQL?

Answer $\mathbf{u}_0$ is the PQL estimate of $\mathbf{u}$. So estimation of β and $\mathbf{u}$ jointly involves maximisation of

$$\frac{\mathbf{y}^T(\mathbf{X}\beta + \mathbf{Z}\mathbf{u}) - \mathbf{1}^T b(\mathbf{X}\beta + \mathbf{Z}\mathbf{u})}{\phi} - \tfrac{1}{2}\mathbf{u}^T\mathbf{G}^{-1}\mathbf{u}.$$

The second term acts as a penalty for the random effects component.

So the thing that we are maximising is a penalised log-likelihood.

For the quasi-likelihood extension we get penalised quasi-likelihood.

i.e. PQL.

Fisher Information

LM	$\frac{1}{\widehat{\sigma_\varepsilon}^2}(\mathbf{X}^T\mathbf{X})^{-1}$
GLM	$\mathbf{X}^T\text{diag}\{b''(\mathbf{X}\widehat{\beta})/\widehat{\phi}\}\mathbf{X}$
LMM	$\mathbf{X}^T(\widehat{\mathbf{R}} + \mathbf{Z}\widehat{\mathbf{G}}\mathbf{Z}^T)^{-1}\mathbf{X}$
GLMM	?

In practice the PQL approximation is often used:

$$\mathbf{X}^T[\text{diag}\{b''(\mathbf{X}\widehat{\beta} + \mathbf{Z}\widehat{\mathbf{u}})/\widehat{\phi}\}^{-1} + \mathbf{Z}\mathbf{G}\mathbf{Z}^T]^{-1}\mathbf{X}.$$

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