17.1.1 Two Restricted Likelihoods That Can't Be Re-expressed

The first example is an additive model with two predictors, x_{1i} and x_{2i}, for the i^{th} observation. Given a spline basis for each predictor, Chapter 4 showed how this model can be written in mixed-linear-model form as

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{Z}_1\mathbf{u}_1 + \mathbf{Z}_2\mathbf{u}_2 + \varepsilon, \tag{17.1}$$

where $\mathbf{X}\beta$ includes the unshrunk parts of the splines for both predictors and $\mathbf{Z}_j\mathbf{u}_j$ contains the shrunk part of the spline for predictor j, so the random effects design matrix in standard form is $\mathbf{Z} = (\mathbf{Z}_1|\mathbf{Z}_2)$. If the spline for predictor j has K_j knots, then the standard-form random effect $\mathbf{u} = (\mathbf{u}_1', \mathbf{u}_2')'$ has covariance matrix

$$\mathbf{G} = \begin{bmatrix} \sigma_{s1}^2\mathbf{I}_{K_1} & \mathbf{0} \\ \mathbf{0} & \sigma_{s2}^2\mathbf{I}_{K_2} \end{bmatrix}. \tag{17.2}$$

To derive the restricted likelihood, let $\mathbf{P}_X^c = \mathbf{I}_n - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}$ be the projection onto the orthogonal complement of the column space of the fixed effect design matrix $\mathbf{X}$. If p is the rank of $\mathbf{X}$, let $\mathbf{H}$ be an $n \times (n-p)$ matrix with orthonormal columns such that $\mathbf{H}\mathbf{H}' = \mathbf{P}_X^c$, e.g., $\mathbf{H}$ has columns equal to the eigenvectors of $\mathbf{P}_X^c$ with eigenvalue 1. Pre-multiply equation (17.1) by $\mathbf{H}'$, so that

$$\mathbf{w} = \mathbf{H}'\mathbf{y} = \mathbf{H}'\mathbf{Z}_1\mathbf{u}_1 + \mathbf{H}'\mathbf{Z}_2\mathbf{u}_2 + \phi. \tag{17.3}$$

Under the usual assumption that $\varepsilon \sim N(\mathbf{0}, \sigma_e^2\mathbf{I}_n)$, $\phi = \mathbf{H}'\varepsilon \sim N(\mathbf{0}, \sigma_e^2\mathbf{I}_{n-p})$. The restricted likelihood is the likelihood for $(\sigma_{s1}^2, \sigma_{s2}^2, \sigma_e^2)$ arising from equation (17.3), so the log restricted likelihood is

$$\begin{aligned} &-0.5\log|\sigma_{s1}^2\mathbf{H}'\mathbf{Z}_1\mathbf{Z}_1'\mathbf{H} + \sigma_{s2}^2\mathbf{H}'\mathbf{Z}_2\mathbf{Z}_2'\mathbf{H} + \sigma_e^2\mathbf{I}_{n-p}| \\ &-0.5\mathbf{w}'(\sigma_{s1}^2\mathbf{H}'\mathbf{Z}_1\mathbf{Z}_1'\mathbf{H} + \sigma_{s2}^2\mathbf{H}'\mathbf{Z}_2\mathbf{Z}_2'\mathbf{H} + \sigma_e^2\mathbf{I}_{n-p})^{-1}\mathbf{w}. \end{aligned} \tag{17.4}$$

To express this restricted likelihood in the desired scalar form, we need to diagonalize three matrices simultaneously: $\mathbf{H}'\mathbf{Z}_1\mathbf{Z}_1'\mathbf{H}$, $\mathbf{H}'\mathbf{Z}_2\mathbf{Z}_2'\mathbf{H}$, and $\mathbf{I}_{n-p}$. To do that, we need to find an orthogonal matrix Γ such that $\Gamma'\mathbf{H}'\mathbf{Z}_1\mathbf{Z}_1'\mathbf{H}\Gamma$ and $\Gamma'\mathbf{H}'\mathbf{Z}_2\mathbf{Z}_2'\mathbf{H}\Gamma$ are both diagonal. Such a Γ exists if and only if $\mathbf{H}'\mathbf{Z}_1\mathbf{Z}_1'\mathbf{H}\mathbf{H}'\mathbf{Z}_2\mathbf{Z}_2'\mathbf{H}$ is symmetric (Graybill 1983, Theorem 12.2.12), which is not true in general. An exercise has you check this.

To ensure that this restricted likelihood has the desired scalar form, a sufficient condition is a form of balance in which the two predictors x_{1i} and x_{2i} are observed on a rectangular grid with the same number of replicates at each grid point. I suspect this is also a necessary condition but I have not proved it. An exercise examines this question.

The second example of a restricted likelihood that can't be re-expressed is the ICAR model with two classes of neighbor relations (2NRCAR) introduced in Section 14.2. (This proof is taken from Reich et al. 2007.) The n-vector $\mathbf{y}$ is modeled as $\mathbf{y} = \delta + \varepsilon$, where $\varepsilon \sim N_n(\mathbf{0}, \sigma_e^2\mathbf{I}_n)$ and δ has an improper normal density specified in terms of its precision matrix:

$$f(\delta|\sigma_{s1}^2, \sigma_{s2}^2) \propto \exp\left[-\frac{1}{2}\delta'\left(\mathbf{Q}_1/\sigma_{s1}^2 + \mathbf{Q}_2/\sigma_{s2}^2\right)\delta\right]; \tag{17.5}$$