REDUCTION OF RESTRICTED
MAXIMUM LIKELIHOOD FOR
RANDOM COEFFICIENT MODELS

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Abstract

The restricted maximum likelihood (REML) estimator of the dispersion matrix for random coefficient models is rewritten in terms of the sufficient statistics of the individual regressions.

KEYWORDS: Restricted Maximum Likelihood, Random Coefficient Models, Structured Linear Regressions, Mixed Models, Estimated Generalized Least Squares
I. Reduction of the Restricted Maximum Likelihood

Restricted maximum likelihood (REML) estimators are widely used to estimate the free parameters in the dispersion matrix for mixed models in structured linear regressions [1, 4–10, 13, 19]. The REML estimator is the maximum likelihood estimate of the parameters which uses only the information not contained in the estimate of the the regression vector, and thereby automatically corrects for the degrees of freedom which are lost in estimating the regression vector.

We consider the subclass of mixed models where the observations are grouped by individual/category, and the observations are uncorrelated across individuals. The resulting covariance matrix has a block diagonal structure. Random coefficient (RC) models are a popular subclass of mixed models where a subset of the regression coefficients varies randomly across individuals [2, 3, 9, 12–21]. In this note, we simplify the REML estimator of the random coefficient model using linear algebra identities. By expressing the likelihood in terms of the sufficient statistics of the individual regressions, the REML degree of freedom correction may be better understood.

A mixed linear model consists of a fixed effects vector, $\alpha$, a fixed effects covariate matrix, $X$, a random effects covariate matrix, $Z$, and three random vectors; the measurement vector, $y$, the measurement error vector, $e$, and the random effects vector, $\beta$, which satisfy the linear equation: $y = X\alpha + Z\beta + e$. We restrict our consideration to linear mixed models with a block structure: $y$, $\beta$ and $e$ consist of $N$ statistically independent subvectors, $y^T = (y_1^T, \ldots, y_N^T)$, $\beta^T = (\beta_1^T, \ldots, \beta_N^T)$ and $e^T = (e_1^T, \ldots, e_N^T)$. We also require $y$, $\beta$ and $e$ to be Gaussian random variables. Thus the $k$th individual, $y_k$, is a Gaussian random variable with the block linear mixed model structure:

$$y_k = X_k\alpha + Z_k\beta_k + e_k,$$

where $X_k$ and $Z_k$ are covariate matrices of dimension $n_k \times p$ and $n_k \times q$ respectively. We allow both $X_k^T X_k$ and $Z_k^T Z_k$ to be singular, and denote their respective ranks by $p_k$ and $q_k$. $e_k$ is a normally distributed random $n_k$-vector of measurement errors with zero mean and covariance $E[e_k e_k^T] = \sigma_k^2 I_{n_k}$, with $\sigma_k^2 > 0$. $\alpha$ is the $p$-vector of fixed effects, and $\beta_k$ is the $q$-vector of random effects. We assume that $\beta_k$ is a zero mean
Gaussian random vector with a \( q \times q \) covariance matrix, \( D(\theta) \), which may be singular. \( \theta \) is an unknown vector that parameterizes \( D(\theta) \), and \( \theta \) is an element in a known, compact, parameter region, \( \Theta \). Thus the covariance of the \( k \)th individual satisfies

\[
\Sigma_k = \sigma^2_k I_{n_k} + Z_k D(\theta) Z_k^t. \tag{2}
\]

We assume that both \( e_k \) and \( \beta_k \) are independent between individuals. We require that \( \sum_{k=1}^N X_k^t \Sigma_k^{-1} X_k \) has full rank. We also assume that the model covariance is identifiable.

We are given a data set consisting of \( N \) distinct individuals, and the measurement vector of the \( k \)th individual, \( \tilde{y}_k \), has \( n_k \) components. \( \tilde{y}_k \) is a realization of \( y_k \), where \( y_k \) has the Gaussian block linear mixed model structure of Eq. (1). Our problem is to infer \( \alpha \) and \( \theta \) conditional on \( \tilde{y}_k \). The maximum likelihood estimator of \( \alpha \) for a fixed value of \( \theta \) is

\[
\hat{\alpha} = \left( \sum_{\ell=1}^N X_\ell^t \Sigma_\ell^{-1} X_\ell \right)^{-1} \sum_{k=1}^N X_k^t \Sigma_k^{-1} \tilde{y}_k, \tag{3}
\]

which has covariance \( \Omega \):

\[
\Omega = \left( \sum_{\ell=1}^N X_\ell^t \Sigma_\ell^{-1} X_\ell \right)^{-1}. \tag{4}
\]

To estimate \( \theta \), we maximize the restricted log likelihood functional as described in [1, 3–9, 12, 13, 19]. For block linear mixed models, the REML functional is given by

\[
\ell(\theta, \hat{\alpha}) = C(N_T - p) + \frac{1}{2} \sum_{k=1}^N \ln(\det (X_k^t X_k)) - \frac{1}{2} \sum_{k=1}^N \ln(\det (\Sigma_k)) - \frac{1}{2} \ln \left( \det \left( \sum_{k=1}^N X_k^t \Sigma_k^{-1} X_k \right) \right) - \frac{1}{2} \sum_{k=1}^N (\tilde{y}_k - X_k \hat{\alpha})^t \Sigma_k^{-1} (\tilde{y}_k - X_k \hat{\alpha}) \tag{5}
\]

where \( \hat{\alpha} \) is given by Eq. (3), \( N_T \equiv \sum_{k=1}^N n_k \), and \( C(N_T - p) \equiv -\frac{1}{2}(N_T - p) \ln(2\pi) \).

On any compact set, the REML estimate of \( \theta \) exists, but may not be unique. Our restriction, that \( \sum_{k=1}^N X_k^t \Sigma_k^{-1} X_k \) is invertible, implies that for any fixed value of \( \theta \), \( \hat{\alpha} \) is unique. Kackar and Harville have proven that any minimum of the REML estimator is an unbiased estimator of \( \alpha \) and \( \beta_k \) [7].

Maximizing \( \ell(\theta) \) in Eq. (5) is often an expensive and ill-conditioned problem. In [16], each individual experiment has hundreds of observations \( n_k \sim 150 \). Using the
standard formulation of Eq. (5), a single descent step requires $O(\sum_k n_k^2)$ operations. In this note, we rewrite Eq. (5) in a computationally convenient form which requires only $O(Np^3)$ operations per step.

To simplify the restricted ML functional, we assume that the column space of $Z_k$ is contained in the column space of $X_k$: $M(Z_k) \subset M(X_k)$, where $M$ denotes the column space. This requirement implies that there are $p \times q$ matrices, $A_k$, such that $Z_k = X_k A_k$. We call this subclass of block linear mixed models, “random coefficient models”. ANOVA models, random constant models with fixed slopes models and the standard formulation of Eq. (5), a single descent step requires $O(\sum_k n_k^2)$ operations. In this note, we rewrite Eq. (5) in a computationally convenient form which requires only $O(Np^3)$ operations per step.

We denote the Moore-Penrose generalized inverse by $\tilde{\cdot}$ and denote the projection onto the column space of a particular matrix, $C$, by $P(C)$: $P(C) \equiv C(C' C)^{-} C'$, and define $P_k \equiv P(X_k)$ When $M(Z_k) \subset M(X_k)$, the estimate of $P_k \alpha$ from the $k$th individual simplifies to the ordinary least squares estimator:

$$\hat{\alpha}_k \equiv (X_k' \Sigma_k^{-1} X_k)^{-} X_k' \Sigma_k^{-1} \tilde{y}_k = (X_k' X_k)^{-} X_k' y_k \ . \quad (6)$$

When $P_k$ is not of full rank, $\hat{\alpha}_k$ estimates only $P_k \alpha$. We define the following matrices: $E_k \equiv (X_k' X_k)^{-}$, $F_k \equiv (Z_k' Z_k)^{-}$, $K_k \equiv E_k X_k' Z_k$, and $L_k \equiv F_k Z_k' X_k$. When $Z_k = X_k$, $K_k$ and $L_k$ are the $p \times p$ projection matrix, $P(X_k' X_k)$. We define the matrix $D_k$ as the projection of $D(\theta)$ onto the column space of $Z_k$:

$$D_k(\theta) = P(Z_k' Z_k) D(\theta) P(Z_k' Z_k) \ . \quad (7)$$

The covariance of the single individual estimate of Eq. (6) is

$$\text{Cov}[\hat{\alpha}_k \tilde{\alpha}_k^t] = (X_k' \Sigma_k^{-1} X_k)^{-} = \sigma_k^2 E_k + K_k D_k K_k^t \ ,$$

where we have used the Sherman-Morrison-Woodbury identity. We define the matrix, $M_k$, to be

$$M_k \equiv X_k' \Sigma_k^{-1} X_k = \sigma_k^{-2} \left( X_k' X_k - L_k' Z_k' Z_k L_k \right) + L_k' [\sigma_k^2 F_k + D_k]^{-} L_k, \quad (8)$$

In deriving Eq. (8), we use the matrix identity:

$$(\sigma_k^2 I_n + Z_k D Z_k)^{-} = \sigma_k^{-2} [I_n - Z_k F_k Z_k'] + Z_k F_k [\sigma_k^2 F_k + D_k]^{-} F_k Z_k' \ . \quad (9)$$

An alternative representation of $M_k$ can be derived by applying the Sherman-Morrison matrix identity [14, p. 33] to Eq. (7). When $Z_k = X_k$, $M_k$ simplifies considerably to $M_k = [\sigma_k^2 F_k + D_k]^{-} = [\sigma_k^2 E_k + D_k]^{-} \ . \quad (10)$
The ML estimate of $\hat{\alpha}$, Eq. (3), may be expressed as the weighted sum of the $N$ individual estimates, $\hat{\alpha}_k$:

$$\hat{\alpha} = \left( \sum_{\ell=1}^{N} (X_{\ell}^t \Sigma_{\ell}^{-1} X_{\ell}) \right)^{-1} \left( \sum_{k=1}^{N} X_k^t \Sigma_k^{-1} \tilde{y}_k \right) = \Omega \sum_{k=1}^{N} M_k \hat{\alpha}_k ,$$

(10)

where $\Omega$, the covariance matrix of $\hat{\alpha}$, satisfies $\Omega = \left( \sum_{k=1}^{N} M_k \right)^{-1}$.

**Theorem:** When $M(Z_k) \subset M(X_k)$, the REML functional of Eq. (5) reduces to

$$\ell(\theta, \hat{\alpha}) = C(N_T - p) + \frac{1}{2} \sum_{k=1}^{N} \ln(\det (X_k^t X_k)) - \frac{1}{2} \sum_{k=1}^{N} (n_k - q) \ln \sigma_k^2$$

$$- \frac{1}{2} \sum_{k=1}^{N} \ln(\det (\sigma_k^2 I_q + Z_k^t Z_k D)) - \frac{1}{2} \ln \left( \det \left( \sum_{k=1}^{N} M_k \right) \right)$$

$$- \sum_{k=1}^{N} \frac{(n_k - p_k) \delta_k^2}{\sigma_k^2} - \frac{1}{2} \sum_{k=1}^{N} (\hat{\alpha}_k - \hat{\alpha})^t M_k (\hat{\alpha}_k - \hat{\alpha}) ,$$

(11)

where

$$(n_k - p_k) \delta_k^2 \equiv \tilde{y}_k^t (I_k - P_k) \tilde{y}_k .$$

**Proof:** We divide the residuals, $\tilde{y}_k - X_k \hat{\alpha} = \tilde{y}_k - X_k \hat{\alpha}_k + X_k (\hat{\alpha}_k - \hat{\alpha})$, into two parts. Since $\tilde{y}_k - X_k \hat{\alpha}_k = (I_{n_k} - P_k) \tilde{y}_k$ is perpendicular to $X_k$, the two parts are independent. From Eq. (9), we have

$$(\tilde{y}_k - X_k \hat{\alpha})^t \Sigma_k^{-1} (\tilde{y}_k - X_k \hat{\alpha}) = (n_k - p_k) \delta_k^2 + (\hat{\alpha}_k - \hat{\alpha})^t M_k (\hat{\alpha}_k - \hat{\alpha}) .$$

(12)

A matrix determinant identity yields

$$\ln(\det (\Sigma_k)) = (n_k - q) \ln \sigma_k^2 + \ln(\det (\sigma_k^2 I_q + Z_k^t Z_k D)) .$$

(13)

□

Thus we have reduced the likelihood function from a function of $N$ matrices of dimension $n_k$ to $N$ matrices of dimension $p$. When the individual variances, $\sigma_k^2$, are given, the likelihood has a simple interpretation as the restricted likelihood of a set of independent regression coefficients with a normal distribution, $\hat{\alpha}_k \sim N(P_k \alpha, \sigma_k^2 E_k + K_k D_k K_k^t)$.
II. Scoring Algorithm

Differentiating the REML function with respect to the $i$th component of $\theta$ yields:

$$\frac{\partial \ell}{\partial \theta_i} = \frac{1}{2} \text{Trace} \left[ \sum_{k=1}^{N} \left( G_k \left( (\hat{\alpha}_k - \hat{\alpha})(\hat{\alpha}_k - \hat{\alpha})^t + \Omega \right) G_k^t - \left( \sigma_k^2 F_k + D_k \right) \right) \right],$$

(14)

where $G_k$ is the $q \times p$ matrix, $G_k \equiv (\sigma_k^2 F_k + D_k)^{-1} F_k Z_k X_k$. When $Z_k = X_k$, $G_k$ simplifies considerably to $G_k = [\sigma_k^2 F_k + D_k]^{-1} = [\sigma_k^2 E_k + D_k]^{-1}$.

From the representation of $\hat{\alpha}$ as the weighted sum of the individual $\alpha_k$, the expectation of the empirical covariance of the random coefficients satisfies

$$L_k \left( E[((\hat{\alpha}_k - \hat{\alpha})(\hat{\alpha}_k - \hat{\alpha})^t) + \Omega_k] \right) L_k^t = D_k + \sigma_k^2 F_k.$$  

(15)

Thus the REML estimate of $D(\theta)$ is a variance weighted version of “total variance = within individual variance + between individual variance.”

By using Eq. (15) to compute $\nabla \theta \ell(\theta, \hat{\alpha}|\tilde{y})$ the operations count is reduced to $O(Np^3)$ per step. Similar savings are achieved in evaluating the Hessian of the REML. A popular maximization technique is the scoring method of Fisher, where $\frac{\partial^2 \ell(\theta, \hat{\alpha}|\tilde{y})}{\partial \theta_i \partial \theta_j}$ is replaced with $E \left[ \frac{\partial^2 \ell(\theta, \hat{\alpha}|\tilde{y})}{\partial \theta_i \partial \theta_j} \right]$. Thus the scoring algorithm is

$$\theta^{\text{new}} = \theta^{\text{old}} + J^{-1} \nabla \theta \ell(\theta^{\text{old}}, \hat{\alpha}|\tilde{y}),$$

(16)

where $J_{i,j} \equiv -E \left[ \frac{\partial^2 \ell(\theta^{\text{old}}, \hat{\alpha}|\tilde{y})}{\partial \theta_i \partial \theta_j} \right] (\theta^{\text{old}}, \hat{\alpha}|\tilde{y})$ with

$$E \left[ \frac{\partial^2 \ell(\theta^{\text{old}}, \hat{\alpha}|\tilde{y})}{\partial \theta_i \partial \theta_j} \right] = \frac{-1}{2} \sum_{k=1}^{N} \text{Trace} \left[ G_k \left( \frac{\partial D_k}{\partial \theta_i} - \frac{\partial \Omega}{\partial \theta_i} \right) G_k \frac{\partial D_k}{\partial \theta_j} \right].$$

(17)

We initialize the scoring algorithm at $\theta = 0$.

Remarks:

1) Swamy [19] has derived the analogous expression for the ML function of the random coefficient model under the assumptions that $Z_k \equiv X_k$ and that the $X_k^t X_k$ are nonsingular.

2) The within individual estimate of $\sigma_k^2$ is

$$\hat{\sigma}_k^2 = \frac{\tilde{y}_k^t P \perp k \tilde{y}_k}{n_k - m_k},$$

(16)
where $P_{\perp k}$ is the projection perpendicular to the extended column space of $(X_k, Z_k)$: $P_{\perp k} \equiv I_{n_k} - P(X_k, Z_k)$, and $m_k$ is the number of degrees of freedom used in the fit, i.e., the rank of $P(X_k, Z_k)$. This estimate is consistent as $n_k \to \infty$.

The REML estimates for $\sigma^2_k$ are noticeably more complicated than the simple within individual least squares estimate of Eq. (16). Hybrid estimation schemes, which utilize the REML Eqs. (10) and (14) to estimate $\alpha$ and $D(\theta)$, and Eq. (16) to estimate $\sigma^2_k$, are of considerable practical interest. This hybrid estimate is empirical Bayesian in $\sigma^2_k$.

3) Since $D(\theta)$ is the variance weighted difference of the empirically estimated covariance of the $\hat{\alpha}_k - \hat{\alpha}$ matrices, and the ordinary least squares estimate of the within individual variance, it can have negative eigenvalues. The standard solution to this problem is to set the negative eigenvalues to zero using the singular value decomposition. This procedure corresponds to imposing a positivity constraint on $D(\theta)$. The constraint produces a slight positive bias in the estimate of $D(\theta)$. The REML estimate of $D(\theta)$ is larger than the ML estimate of $D(\theta)$, and thus the REML correction reduces the probability of negative eigenvalues, but does not eliminate it.

4) When data are missing, the expected maximization (EM) algorithm may be applied to Eqs. (10), and (14) directly just as the EM algorithm has been applied to the original REML formulation [9, 10, 12, 13, 19].

5) The REML estimator does not directly use estimates of the random effects, $\beta_k$, nor does it yield estimates of $\beta_k$. However, the random effects may be estimated from $\hat{\beta}_k = D_k Z_k^t \Sigma_k^{-1} (\tilde{y}_k - X_k \hat{\alpha}) = D_k [\sigma^2_k F_k + D_k]^{-1} L_k (\hat{\alpha}_k - \hat{\alpha})$, which is both the best linear unbiased estimator when $\theta$ is known and the empirical Bayesian estimator when $\theta$ is estimated from Eq. (11).

III. Conclusion

The restricted maximum likelihood estimator for the dispersion matrix of random effects models requires only the ordinary least squares estimates for each separate individual and the corresponding covariance matrices of the individual estimates. Thus we have reduced the computational cost per descent step from $O(\sum_k n_k^3)$ operations to $O(Np^3)$ operations per step.
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