Application of Householder's transformations and the QL algorithm to REML estimation of variance components

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Restricted maximum likelihood (REML) is widely regarded as the preferred procedure for estimating variance components in animal breeding problems. The size of the coefficient matrix, however, often leads to computational difficulties and many simplified algorithms, including diagonalization, have been proposed. Diagonalization of the mixed model equations coefficient matrix, augmented by the numerator relationship matrix, in different steps using Householder's transformations and the QL algorithm is proposed. The transformations need only be performed once. Very large data sets can be handled with ease and once the transformations have been performed, there is no practical limitations to the number of iterations that may be performed. A numerical example illustrating the procedure is supplied and a FORTRAN program, based on this approach, is available.

Keywords: Diagonalization, restricted maximum likelihood, variance components.

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Introduction

Estimation of (co)variance components plays an important role in animal breeding research since these components are used in the estimation of genetic parameters and the selection of a design for an animal breeding programme. In recent years, restricted maximum likelihood (REML) of Patterson & Thompson (1971) has become the method of choice, the reason being the desirable properties of REML estimators as discussed by Harville (1977) and the fact that REML yields estimates of variance components free of selection bias (Henderson, 1986). Although many improved algorithms for REML estimation of variance components have been published (Harville & Callanan, 1990), it is still regarded as computationally demanding especially for large data sets. To simplify the computations, Patterson & Thompson (1971) have suggested diagonalization of the coefficient matrix of the mixed model equations (MME). Another approach used by Smith & Graser (1986) was tridiagonalization of the MME coefficient matrix, so that direct inversion is not necessary. Although Lin (1987; 1988) has presented further simplifications, this is still an area for further research. The purpose of this study is to present computational algorithms for diagonalization of the MME coefficient matrix augmented by the numerator relationship matrix A, leading to an efficient algorithm for REML variance components estimation.

Procedures

Consider a univariate mixed linear model with one random factor. Let y, b, u and e denote the vectors of observations, fixed effects (and possible covariates), random effects, and residual error, respectively. X and Z are design matrices, for fixed and random effects and X may also contain columns for covariates. The general linear mixed model can be written as follows:

\[ y = Xb + Zu + e \]  

with \( E(y) = Xb, \ E(u) = 0, \ Var(u) = G, \ Var(e) = R, \ Var(y) = GZ\alpha + R \) and \( Cov(u,e) = 0 \). In most applications \( G = A\sigma^2_u \) where \( A \) describes the covariance structure among the levels of the random factor and \( R = I\sigma^2_e \).

In animal breeding terms, assuming an additive genetic model for the random factor (sires), \( A \) is the numerator relationship matrix. The mixed model equations (MME) of Henderson (1973) are then:

\[
\begin{bmatrix}
X'X & X'Z \\
Z'X & Z'Z + A^{-1}\alpha
\end{bmatrix}
\begin{bmatrix}
b \\
\alpha
\end{bmatrix}
= 
\begin{bmatrix}
X'y \\
Z'y
\end{bmatrix}
\]  

(2)

with \( \alpha = \sigma^2_u / \sigma^2_e \), assuming that \( \sigma^2_e \) and \( \sigma^2_u \) are known parameter values. Since they are never known, estimates can be obtained from the data available. Restricted maximum likelihood (REML) accounts for the loss of degrees of freedom due to fitting the fixed effects. Maximization of the part of the likelihood of the data vector \( y \), which is independent of the fixed effects, is achieved by operating on a vector of 'error contrasts', \( Sx \), with \( SX = 0 \), and \( E(Sy) = 0 \). A suitable matrix arises when fixed effects (and possible covariates) are
absorbed into the random effect in (2) (Thompson, 1973; Meyer, 1987). After absorption, the MME become

\[ (Z'SZ + \alpha A^{-1})u = Z'Sy \tag{3} \]

with \( S = I_n - X(X'X)^{-1}X' \). Then \( \sigma_u^2 \) and \( \sigma_\ell^2 \) can be estimated by iteration on:

\[ \hat{\sigma}_u^2 = \frac{[y'y - \bar{u}'Z'Sy]}{[N - r(X)]} \tag{4} \]

\[ \hat{\sigma}_\ell^2 = \frac{[u'AI - \hat{\sigma}_u^2 + \hat{\sigma}_\ell^2 tr (A^{-1}(Z'SZ + \alpha A^{-1}))]}{q} \tag{5} \]

where \( N \) = total number of observations, \( r(X) \) = rank of \( X \), \( tr \) = trace of a matrix, and \( q \) = number of levels for the random factor (sires). Equivalent expressions of (4) and (5) are given by Harville (1977), Searle (1979), Henderson (1984) and Meyer (1987).

Only first derivatives of the likelihood function are utilized by eqns. (4) and (5), which result in an expectation maximization (EM) algorithm of Dempster et al. (1977; 1984). Apart from the slow convergence of the EM algorithm, and the problem of convergence to a global vs. local maximum, it is in many practical situations difficult and sometimes impossible to use formulae (4) and (5) because of the large coefficient matrix in (3).

Lin (1988) has proposed four alternative algorithms in an attempt to solve the problem. One of these algorithms uses an orthogonal matrix \( U \) which simultaneously diagonalizes \( Z'SZ \) and \( A^{-1} \) in (3). This approach is very useful for small data sets but, with large data sets, it becomes impractical because the matrix \( U \) is too large to fit in the memory of most computers. An alternative approach for diagonalization of the coefficient matrix in (3) can be used following several computational steps. The numerator relationship matrix \( A \) can be decomposed by the method of Cholesky as \( LL' \). Then \( \text{Var}(y) = ZLL'Z\sigma_u^2 + \sigma_\ell^2 \). Thus, if we define

\[ Z_i = ZL_i \]

an equivalent model to (1) is \( y = Xb + Z_iu_i + e \), where \( u_i = L^{-1}u \), \( \text{Var}(u_i) = \sigma_u^2 I \) and \( \text{Var}(y) = Z_iZ_i^t\sigma_u^2 + \sigma_\ell^2 I \).

MME equations become

\[ (L'Z'SZL + \lambda\alpha)L^{-1}u = L'Z'Sy \ . \tag{6} \]

Because \( L'Z'SZL \) is symmetric, there exists an orthogonal matrix \( K \) such that \( K'(L'Z'SZL)K = D = \text{diag} (\lambda_1, \lambda_2, \ldots, \lambda_n) \), for \( i = 1, \ldots, n \), \( \lambda \) being the eigenvalues of \( L'Z'SZL \) (Graybill, 1976; Searle, 1982; Golub & Van Loan, 1983). There are different methods of obtaining \( K \), but one of the most efficient algorithms is a combination of Householder’s transformations and the QL algorithm (Wilkinson, 1978; Wilkinson & Reinsch, 1971). Any real symmetric matrix may be reduced to tridiagonal form using Householder’s method (Wilkinson & Reinsch, 1971). According to Martin et al. (1971), \( L'Z'SZL \) can be reduced to a tridiagonal symmetric matrix as follows:

\[ (L'Z'SZL)_{i+1} = P_i(L'Z'SZL),P_i \quad \text{for} \ i = 1, 2, \ldots, n-1 \tag{7} \]

where the \( P_i \) are Householder transformation matrices of the form

\[ P_i = I - u_iu_i' / H_i \quad \text{with} \ H_i = \frac{1}{2} u_iu_i', \quad \text{for} \ u'u = 1 \tag{8} \]

The right-hand sides in (6) can be transformed using the structure of the \( P_i \) matrices, e.g.

\[ (L'Z'S)y_{i+1} = P_i(L'Z'S)y_i = (L'Z'S)y_i - u_if / H_i \tag{9} \]

where \( f = u_i'(L'Z'S)y_i \). Note that \( f \) is a scalar, so the transformation of the RHS in (6) can easily be accomplished during the process of the formation of an element of \( P_i \).

The next step is to find the eigenvalues of the coefficient matrix in (6). One of the most elegant methods is the QL algorithm described by Bowdler et al. (1971). When the matrix is symmetric and tridiagonal as in (7), there exists a matrix \( Q \) such that

\[ [P'(L'Z'SZL)P]_{i+1} = Q_i[P'(L'Z'SZL)P]_iQ_i \tag{10} \]

and \( Q_i \) is obtained in the factorized form as

\[ Q_i = T^{(0)}_i, T^{(0)}_i, \ldots, T^{(0)}_i \tag{11} \]

with \( T^{(0)}_i \) determined in the order \( T^{(0)}_i, \ldots, T^{(0)}_i \); \( T^{(0)}_i \) being a rotation in the \((i,i+1)\) plane, designed to annihilate the \((i,i+1)\) element. If we write

\[ T^{(0)}_i = \begin{pmatrix} 1 & & & \\ & c_i & -s_i & \\ & s_i & c_i & \\ & & & 1 \end{pmatrix} \quad \begin{pmatrix} 1 \\ c_i \\ -s_i \\ s_i \\ c_i \end{pmatrix} \]

then (10) can be rewritten as \[ P'(L'Z'SZL)P)_{i+1} = M_iT^{(0)}_i \ldots T^{(0)}_i \tag{12} \]

After post-multiplication of \( M \) by \( T^{(0)}_i \ldots T^{(0)}_i \), there is only one super-diagonal line of non-zero elements, and Bowdler et al. (1971) have shown that there is no need to form \( M \) explicitly. As the \( T \) matrices have a simple structure, the RHS in (9) can be easily transformed as has been suggested by Wilkinson (1978). Let \( P'L'Z'Sy = z \). Then calculate

\[ t_i = z_s - sz_{i+1} \tag{13} \]

\[ t_{i+1} = z_s + ct_{i+1} \tag{14} \]

and overwrite \( t_i \) and \( t_{i+1} \) on \( z_i \) and \( z_{i+1} \).

From (6) we can obtain estimates for \( \sigma_u^2 \) and \( \sigma_\ell^2 \) as follows:

\[ \hat{\sigma}_u^2 = \frac{[y'y - \bar{u}'Z'Sy]}{[N - r(X)]} \tag{15} \]

\[ \hat{\sigma}_\ell^2 = \frac{[u'I - \hat{\sigma}_u^2 + \hat{\sigma}_\ell^2 tr (A^{-1}(Z'SZ + \alpha A^{-1}))]}{q} \tag{16} \]

Proof of the equivalence between (4), (5), (15), and (16) can be found in Lin (1988).

Proof that direct matrix inversion and the described diagonalization approach are identical, is now supplied: The matrix \( P \) arising from Householder’s transformations is orthogonal as well as the matrix \( Q \) from (10) (Wilkinson, 1978).

Let \( K = PQ \). The matrix \( K \) is also orthogonal (Wilkinson, 1978; Searle, 1982). By definition:

\[ K'(L'Z'SZL + \lambda\alpha)K = D + \lambda\alpha \]

\[ L'Z'SZL + \lambda\alpha = K^{-1}(D + \lambda\alpha)K^{-1} \]

\[ (L'Z'SZL + \lambda\alpha)^{-1} = K'(D + \lambda\alpha)^{-1}K \tag{17} \]

It is obvious from (17) that

\[ tr[(L'Z'SZL + \lambda\alpha)^{-1}] = tr[(D + \lambda\alpha)^{-1}] \]

Since \( (D + \lambda\alpha) \) is diagonal, the calculation of the trace of its inverse is trivial.
Now the variance components can be estimated by iteration on:
\[ \hat{\sigma}_a^2 = \frac{[y' Sy - \hat{u^*}' t]}{[N - r(X)]} \quad (18) \]
\[ \hat{\sigma}_e^2 = \frac{\hat{u^*}' \hat{u^*} + \hat{\sigma}_a^2 \text{tr}(D + \lambda \lambda')}{q} \quad (19) \]
where \( \hat{u^*} = K'L^{-1}u \) is a solution vector to the diagonalized system and \( t = K'L'Z'Sy \) is the vector of transformed RHS.

The proposed algorithm for REML estimation of variance components can be summarized as follows:

(a) Absorb the fixed effects (and possible covariates) into the random effect of the model. This can be done using Gaussian elimination or SWEEP techniques described by Goodnight (1979).

(b) Calculate \( L \), a lower triangular matrix of the numerator relationship matrix by the indirect method proposed by Henderson (1976). Premultiply both sides of (3) by \( L' \) and postmultiply left-hand side by \( L \) to obtain (6). This step can be skipped if the recursive algorithm of Quaas (1989) is used which directly overwrites (3) by \( L \) to obtain (6) without computing \( L \) explicitly.

(c) Calculate \( K'(L'Z'SZL)K = D \) and \( K'L'Z'Sy = t \).

(d) Calculate \( \hat{u^*} = (D + \lambda \lambda')^{-1}t \).

(e) Calculate \( \hat{\sigma}_a^2 \) and \( \hat{\sigma}_e^2 \) according to (18) and (19). Steps (a) to (d) are to be performed only once, before the iteration process.

Repeat calculations for \( \hat{\sigma}_a^2 \) and \( \hat{\sigma}_e^2 \) until convergence of REML is achieved.

### Numerical example

The sample data used are supplied in Table 1. The model used for analysis contained ten herd-year-season fixed subclasses, age of dam as independent variable and nine sires as the random factor. The trait is average daily gain of Dormer lambs.

The nine sires were assumed related but non-inbred and the numerator relationship matrix \( (A) \) is given in Table 2.

### Table 1 Data for numerical example

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<th>1</th>
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<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
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<td>0</td>
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<tr>
<td>( y_{.i.} )</td>
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<td>( n_{.i.} )</td>
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</table>

The least squares equations after absorption of the fixed effects into the sire effect, e.g. \( Z'SZu = Z'Sy \) are given in (18).

### Table 2 Numerator relationship matrix \( (A) \) for the nine sires

\[
\begin{array}{ccccccccccc}
1 & 0 & 0 & .5 & .5 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & .5 & .5 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & .5 & .5 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & .5 & .5 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & .5 & .5 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & .5 & .5 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & .5 & .5 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & .5 & .5 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & .5 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\end{array}
\]

\[
\begin{array}{ccccccccccc}
\text{symmetric} & 1 & .25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\text{symmetric} & 1 & .25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]
When $A^{-1}$, multiplied by the ratio $\sigma_2^2/\sigma_9^2 = 33$ is added to $Z'SZ$ and the direct inversion approach is applied, the following results are obtained:

\[ \hat{u}'A^{-1}\hat{u} = 376.4237 \]

\[ tr[A^{-1}(Z'SZ + 33.6918A^{-1})^{-1}] = 0.1513 \]

\[ \hat{u}'Z'Sy = 32139.4394 \]

The lower triangular matrix $(L)$ of numerator relationship matrix $(A)$ and $L'Z'SL$ and $L'Z'Sy$ are given in (19) and (20), respectively.

The tridiagonal matrix $P'L'Z'SLP$ and corresponding RHS, $P'L'Z'Sy$ after Householder's transformations are given in (21).

Finally, the diagonal matrix and corresponding RHS after QL transformation are given in (22).

The results are identical to those obtained by direct inversion approach, e.g.

\[ \hat{u}'u* = 376.4237 \]

\[ tr(D + \lambda I)^{-1} = 0.1513 \]

\[ \hat{u}'t = 32139.4394 \]

When the data from the numerical example are used, after 95 iterations, $\sigma_2^2 = 2592.9615$ and $\sigma_9^2 = 115.0857$.

\[
\begin{array}{cccccccccc}
1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 1.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 1.0000 \\
\end{array}
\]

(19)

\[
\begin{array}{cccccccccc}
56.9637 & -17.4119 & -11.9198 & -1.3205 & 17.1140 & 9.4515 & -10.8778 & -7.2276 & 0 & 0 \\
58.4125 & -18.6085 & -8.5003 & -3.2133 & -0.446 & 0.517 & 0 & 0 & 0 & 0 \\
36.5126 & -2.9555 & 0.265 & -0.0374 & 0.434 & 0 & 0 & 0 & 0 & 0 \\
46.6434 & -14.487 & -10.8340 & -7.0159 & 0 & 0 & 0 & 0 & 0 & 0 \\
31.078 & -8.3220 & -5.1376 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
26.1983 & -6.8797 & 18.8446 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]

(20)

\[
\begin{array}{cccccccccc}
51.6307 & 7.3564 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
7.3564 & 6.5524 & 12.264 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 12.264 & 57.2303 & 15.0102 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 15.0102 & 71.4340 & -18.1916 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -18.1916 & 56.7078 & -16.8282 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -16.8282 & 19.3432 & -8.8876 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -8.8876 & 58.2629 & -42.9978 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -42.9978 & 54.1890 & 14.9842 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 14.9842 & 18.8446 & 0 \\
\end{array}
\]

(21)

\[
\begin{array}{cccccccccc}
116.3470 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 101.0568 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 60.6445 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 52.4040 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 30.7694 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 23.8769 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 6.4379 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.6586 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]

(22)
Discussion

Both the theoretical development and the numerical example have shown that direct inversion and a diagonalization approach using Householder’s transformations and the QL algorithm yield identical results. Simplification of the absorbed MME coefficient matrix by changing coordinates to an eigenbasis has been noted by Patterson & Thompson (1971) and Olsen et al. (1976). However, finding the eigenvalues of a large matrix is not a trivial problem. It is suggested that this should be done in two steps. Firstly, the coefficient matrix is to be reduced to tridiagonal form through the series of Householder’s transformations. The reason for having chosen this method is that it is more economical with respect to the arithmetic involved (Golub & Van Loan, 1983), and gives very stable reductions (Martin et al., 1971). The procedure ‘tred3’ of Martin et al. (1971) was chosen after it had been rewritten from ALGOL to FORTRAN. It has also been modified to perform transformations on the RHS as shown in (9). The second step used in the proposed diagonalization approach was to find the eigenvalues of the tridiagonal matrix obtained using Householder’s transformations. The QL algorithm proposed by Bowdler et al. (1971) was suggested because of its simplicity and well-known properties. Their QL procedure ‘qul’ was rewritten in FORTRAN and modified to transform the RHS as showed previously.

The proposed diagonalization approach is very efficient, because both Householder’s and QL transformations must be performed only once. The rest of the computations at each round of iteration of the EM procedure are reduced dramatically, because the coefficient matrix is diagonal. This leads to an important advantage in that there is no practical limit to the number of iterates that may be performed. A FORTRAN program for REML estimation of variance components by this diagonalization approach is available on request from the authors.

References


