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Application of F-G Diagonalization Algorithm to Restricted Maximum Likelihood Estimation of Variance Components

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Abstract. The F-G algorithm of Flury and Gautschi can be used to find an orthogonal matrix B such that:

$$\phi(B) = \prod_{i=1}^{k} \{\det[\mathrm{diag}(B'CiB)]/\det(Ci]\}^{n_i}$$

is minimum, where C_i is $(Z'MZ + \propto A^{-1})$ and $n_1 \ldots\ldots, n_k$, are positive weights. The orthogonal matrix B can be interpreted as the matrix which brings matrices $C_1 \ldots\ldots,$ C_k simultaneously as close to diagonality as possible. To reduce the number of operations required by F-G algorithm, Clarkson used a modified algorithm (MF-G) to find an orthogonal matrix B such that $B'C_iB$ is nearly diagonal. Both F-G and MF-G algorithm were applied to three sets of mixed model coefficient matrices in animal breeding cases. Close estimate to the exact REML solutions were obtained for traits with low heritability (large $\propto$). One can use equal or unequal weights $n_1, \ldots\ldots, n_k$ to achieve convergence for both algorithms.

Introduction

Variance component estimation can be very demanding computationally for large data set. Restricted maximum likelihood (REML) was derived by Patterson and Thompson [1] whose purpose was to eliminate the bias in maximum likelihood (ML) due to estimation of fixed effects. Smith and Graser [2] described an efficient algorithm for computing REML estimators of variance components in a class of mixed model. They tridiagonalized the coefficient matrix through a series of Householder transformations so that direct inversion of the coefficient matrix was unnecessary. They found that evaluation of $\mathrm{tr}(Z'MZ+\propto I)^{-1}$ is the most computationaly demanding step in the tridiagonalization procedure. However, computing this trace becomes a computational triviality using procedure through singular value decomposition. Since $(Z'MZ+\propto I)$ and $(D+\propto I)$ are similar matrices where $D=V'(Z'MZ)V$ and V is an orthogonal matrix and, hence, $tr(Z'MZ+\propto I)^{-1} = (D+\propto I)^{-1}$. So $Tr(Z'MZ+\propto I)^{-1}$ is simply the sum of the reciprocals of the diagonal elements of the matrix $(D+\propto I)$.

In animal breeding, if the sires are related with a relationship matrix (A), Smith and Graser [2] suggested to redefine Z_1 as ZL such that $A = LL'$ where L is the lower triangular matrix obtained by applying Cholesky Decomposition to A. So $(Z'_1MZ+\propto I)s^*=Z_1MY$ where $M=I-X'(X'X)^{-1}X$ and $s^*=L^{-1}s$.

Patterson and Thompson [1] and Thompson and Cameron [3] suggested the diagonalization of the coefficient matrix $(Z'MZ+\propto I)$ to reduce the CPU time required to obtain direct inverse in each iteration. Their basic idea was to calculate the inverse of $(Z'MZ+\propto I)$ by computing $V(D+\propto I)^{-1}V'$ instead of direct inversion because $(Z'MZ+\propto I)^{-1} = V(D+\propto I)^{-1}V'$. Computation of $V(D+\propto I)^{-1}V'$ consumes less CPU time than direct inversion mainly because $(D+\propto I)$ is a diagonal matrix. Although this diagonalization procedure reduces computational time compared to the direct inversion approach, it still involves the calculation of $V(D+\propto I)^{-1}V'$ in each iteration.

Lin [4] applied singular value decomposition to the coefficient matrix of mixed model equations and used orthogonal matrix V to diagonalize Z'MZ. Although diagonalization of Z'MZ involves extensive calculations compared with matrix inversion, it needs to be done only once independently of the number of iterations. After diagonalization, obtaining solutions and estimating variance components are all trivial calculations regardless of the number of iterations, whereas direct inversion approach needs to invert the coefficient matrix in each iteration. Thus Lin's technique will undoubtedly result in a substantial reduction in CPU time compared with the direct inversion approach or the approach of Patterson and Thompson [1].

Lin and Smith [5] applied FG algorithm to transform a multitrait into a unitrait mixed model that has equal design matrices for t traits and contains more than one random effect. The class of models was restricted to those in which the covariance matrices for all random effects including the residual can be diagonalized simultaneously.

All previous studies agreed that inversion of $(Z'MZ+\propto I)$ is a computational demanding in calculating solution of random effects or in computing REML estimators of variance components. Appropriateness of an algorithm may change depending on the size of the data and computer capacity.

The purpose of this study is to present nearly simultaneous diagonalization algorithms (F-G and MF-G) as proposed by [6-8] and apply them to the coefficient matrices of mixed models estimate REML variance components.

Materials and Methods

Statistical Model

The mixed linear model that has been used in animal breeding is the following: $y = Xb+Zu+e$ where

- y is an $n*1$ data vector of a trait.
- X is a known, fixed $n*p$ matrix with $\text{rank}=r \leq \min(n,p)$.
- b is a fixed unknown vector.
- Z is a known incidence $n*q$ matrix.
- u is a nonobservable $q*1$ random vector (say sire).
- e is a $n*1$ nonobservable random vector.

$E(u)=E(e)=O$, $V(u)=Ae_u^2$ if A^{-1} (inverse of numerator relationship matrix) is used, otherwise $V(u)=I\sigma_u^2$; $V(e)=I\sigma_e^e$ [9, p.16].

The mixed-model equations (MME) of Henderson [9] are:

$$\begin{bmatrix} X'X & X'Z \\ Z'X & Z'Z+\propto I \end{bmatrix} \begin{bmatrix} \hat{b} \\ \hat{u} \end{bmatrix} \begin{bmatrix} X'Y \\ Z'Y \end{bmatrix}$$

After absorption of the fixed effects, Henderson's mixed model equations will be $(Z'MZ+\propto I)\hat{u} = Z'MY$ where $M=I-X'(X'X)^{-1}X$

and $\propto = \dfrac{\hat{\sigma}_e^2}{\hat{\sigma}_u^2}$

Thus $\hat{u} = C^{-1}Z'MY$ and $C = (Z'MZ+\propto I)$, C has the order of q sires and is difficult to compute if q is large.

The REML estimates of sire and error variance components were:

$$\hat{\sigma}_e^2 = [Y'MY - u'(Z'MY)]/[N - \text{rank}(x)]$$

$$\hat{\sigma}_u^2 = u'u + \hat{\sigma}_e^2 \,\text{tr}\,(Z'MZ + \propto I)^{-1}\,]/q,$$

where N is the number of observations and q is the number of sires.

F-G or MF-G algorithms can be applied to diagonalize simultaneously coefficient matrices of mixed model equations. The simplified procedure in calculating REML variance components can be summarized as follows:

1. Accumulate the coefficient matrices $C_1, \ldots, C_k$ and $P_1, .. P_k$, where each C can be one of the form of $Z'MZ$, $(Z'MZ + \propto I)$ or $(Z'MZ + \propto A^{-1})$ and each P_i is in the form $P_i = Z'MY$
2. Apply F-G or MF-G algorithms on each C_i, each with dimension q^*q to obtain the orthogonal matrix B.
3. Compute $B'C_iB$ and $B'Z'MY$.
4. One can apply Gaussian elimination to get an exact solution or create a diagonal matrix $D_i = \text{Diag}\,(B'C_i\,B)$ to compute approximate solution.
5. Examine closeness to diagonality by
   a) comparing the diagonal elements and the eigenvalues of the transformed matrix.
   b) Computing $Q(B) = \det\{\text{Diag}(B'C_i\,B)\}/\det(C_i)$
6. Solve for $u^* = (D_1 + \propto I)^{-1} B'Z'MY$.
7. Compute $\text{tr}(Z'MA + \propto I)^{-1}$, u^*u^* and $u^*Z'MY$.

F-G algorithm

Flury and Gautschi [6] found that for given $k > 1$, positive definite p^*p matrices $C_1 \ldots\ldots, C_k$ and k positive integers $n_1, \ldots\ldots n_k$. the algorithm finds an orthogonal matrix B such that:

$$\Phi\,(B) \prod_{i=1}^{k} [\det(\text{diag}(B'C_iB)/\det(C_i)]^{n_i} \text{ is minimum} \tag{1}$$

The matrix B brings matrices $C_1 \ldots\ldots, C_k$ simultaneously as close to diagonality as possible. Flury [10] showed by using the maximum likelihood estimation of common principal axis in k normal populations that

$\Phi(B)$ is minimum if the following system of equations holds:

$$b_l \left(\sum_{i=1}^{k} n \frac{E_{il} - E_{ij}}{E_{il} E_{ij}} C_i \right) b_j = 0, \ (l,j=1, \ldots, p; l=j) \qquad (2)$$

where

$$E_{ih} = b_h' C_i b_n \ (i = 1, \ldots\ldots, k; \ h=1, \ldots\ldots, p) \qquad (3)$$

The F-G algorithm consists of two subroutines, called F and G respectively, which minimize $\Phi(B)$ by iteration on two levels: on the outer level (F-level) every pair (b_1, b_j) of column vectors of the current approximation B to the solution B is rotated, such that equation (3) is satisfied. One iteration step of the F-algorithm consists of rotation of all $p(p-1)/2$ pairs of vectors of B. On the inner level (G-level), an orthogonal, 2*2 matrix, Q which solves a two dimensional analog of (3), is found by iteration. This matrix defines rotation of a pair of vectors currently being used on the F-level, Flury and Gautschi [6, p.171,172].

Clarkson [8] modified the F level of F-G algorithm and improved its performance by reducing the number of operations required for each pair of orthogonal column vectors $B_p = (b_j, b_l)$ in B. An orthogonal matrix P is found such that:

$$P = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$$

where c and s are the sin and cosin of the rotation angle $(c^2 + s^2 = 1)$. Given c, the updated versions of vectors b_j, b_l are computed as $B^n = B_p P$, that is $b_j^n = cb_j + sb_l$ and $b_l^n = -sb_j + cb_l$ updated vectors.

In Flurry and Gautschi [6] algorithm, maximum likelihood estimates for C were found via the "G" step by use of k matrices Ti, where $T_i = b_j, b_l) C_i' b_j b_l)$. Roughly $2kp^2$ operations are required to obtain all k matrices T_i for one F step. Since each F iteration must consider all $p(p-1)/2$ possible pairs of vectors (b_l, b_j), the order of kp^4 operations are required in each F iteration in computing the T_i's. This is the maximum number of operations required by any phase of the F-G algorithm. In MF-

G algorithm, the k multiplication is not utilized in computing T_i,s resulting in a significant increase in performance of the algorithm, Clarkson [8,p.148-149] F-G algorithm, KP^3 operations are required per F iteration to update the matrices. T_i's.

Numerical Example

Table 1. Example data were adapted from Schaeffer [11].

Herd-year-Season	Sire eartage	No. of progeny	Total yield/100
1	1	4	531
1	2	3	449
1	3	3	416
2	2	3	411
2	4	2	298
3	3	4	624
3	5	6	983
4	1	2	302
4	6	3	526
5	1	2	321
6	1	2	254
6	4	4	746
6	6	2	363

The model used for analyzing the data contains the fixed effect of herd-year-season and random effect of sire. After absorbing the fixed effect and assuming $\propto = 15$ the coefficient matrix is

1) With unrelated sires (say base population):

$$Z'MZ+\propto I=\begin{bmatrix} 5.1 & -1.2 & -1.2 & -1.0 & 00.0 & -1.7 \\ -1.2 & 3.3 & -.9 & -1.2 & 00.0 & 00.0 \\ -1.2 & -.9 & 4.5 & 00.0 & -2.4 & 00.0 \\ -1.0 & -1.2 & 00.0 & 3.2 & 00.0 & -1.0 \\ 00.0 & 00.0 & -2.4 & 00.0 & 2.4 & 00.0 \\ -1.7 & 00.0 & 00.0 & -1.0 & 00.0 & 02.7 \end{bmatrix} +15^{*}I_6$$

$$(Z'MY)' = (-143.35\ \ 15.80\ -21.60\ \ 78.90\ \ 18.80\ \ 51.45$$

2) With related sires (say first generation):

If the relationship matrix among sires, A is

$$A = \begin{bmatrix} 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 1.000 & 0.500 & 0.750 & 0.750 & 0.750 \\ 0.000 & 0.500 & 1.000 & 0.750 & 0.750 & 0.750 \\ 0.000 & 0.750 & 0.750 & 1.250 & 0.750 & 1.000 \\ 0.000 & 0.750 & 0.750 & 0.750 & 1.250 & 1.000 \\ 0.000 & 0.750 & 0.750 & 1.000 & 1.000 & 1.375 \end{bmatrix}$$

$Z_1'MZ_1 = L'Z'MZL$ and L is a lower triangular matrix such that $A = L'L$

$$Z_1'MZ_1 + \ :I = \begin{bmatrix} 5.000 & -3.825 & -2.208 & -1.308 & -.601 & -1.041 \\ -3.825 & 3.469 & .617 & .769 & .875 & .781 \\ -2.208 & .617 & 2.756 & .934 & -.475 & .451 \\ -1.308 & .769 & .934 & 1.438 & .088 & .152 \\ -\ .601 & .875 & -.475 & .088 & 1.538 & .585 \\ -1.041 & .781 & .451 & .152 & .585 & 1.013 \end{bmatrix} + 15^*I_6$$

F-G and MF-G algorithms were applied on different sets of coefficient matrices:

1) $Z'MZ$ and $Z_1'MZ_1$ where $Z_1' = L'Z'$.
2) $(Z'MZ+\propto I)$ and $(Z_i'MZ_i + \propto I)$.
3) $(Z'MZ+\propto I)$ and $(Z_1'MZ_1 + \propto A\text{-}1)$.

These three sets were chosen as an example to demonstrate simultaneous diagonalization of two coefficient mixed model matrices. Moreover, each set will differ from the other in the magnitude of the diagonal and off-diagonal elements.

Different values of $\propto = 15, 50$ and 500 were used. An initial matrix B=I and equal and unequal weights were used in F-G and MF-G to compute an orthogonal matrix B which diagonalizes each set. The matrix B which achieves near diagonality for $\propto =$ 15 for each set is:

$$B_1 = \begin{bmatrix} .7063 & .6302 & .2524 & .1520 & .0417 & .1247 \\ -.5732 & .7765 & -.2048 & -.1234 & -.0338 & -.1012 \\ .3126 & .0000 & .9457 & -.0673 & -.0184 & -.0552 \\ -.2035 & .0000 & .0000 & -.9783 & -.0120 & -.0359 \\ -.0571 & .0000 & .0000 & .0000 & .9983 & -.0101 \\ -.1739 & .0000 & .0000 & .0000 & .0000 & .9848 \end{bmatrix}$$

$$B_2 = \begin{bmatrix} .7756 & .5406 & -.0182 & -.1697 & -.0865 & -.2636 \\ -.5135 & .3068 & -.4031 & -.3400 & -.1857 & -.5740 \\ -.2694 & .3601 & .753 & -.2439 & .4057 & -.0821 \\ -.1743 & .3882 & .1891 & .8000 & -.3562 & -.1280 \\ -.0596 & .3614 & -.4764 & .2772 & .7274 & .1815 \\ -.1679 & .4502 & -.0863 & -.2816 & -.3708 & .7382 \end{bmatrix}$$

$$B_3 = \begin{bmatrix} .9861 & .1497 & .0089 & .0257 & .0666 & -.0055 \\ -.0618 & .3878 & -.3696 & -.6244 & .2930 & -.4832 \\ -.0024 & .4567 & .5241 & -.3064 & -.6492 & -.0291 \\ -.0554 & .3872 & -.3443 & .6610 & -.2953 & -.4521 \\ -.1262 & .4701 & .5331 & .2798 & -.6329 & -.0078 \\ -.0657 & .4977 & -.4313 & -.0185 & -.0206 & -.7491 \end{bmatrix}$$

Flury [10] and Flury and Gautschi [6] found the eigenvectors of the diagonalizable matrices, but B can be considered as "compromises" between the eigenvectors of the untransformed matrices.

Tables 2 and 3 show that the trace, u′u and u′Z′MY of the three sets of transformed matrices are approximate to those of exact solution (direct inversion). Diagonalization of $(Z'MZ+\propto I)$ and $(Z_1MZ_1+\propto I)$ gave the nearest results to the exact solution. Dropping the off-diagonal elements from the transformed matrices gave approximate variance components of REML (Tables 2 and 3). One can get the exact solution by inverting the complete transformed matrices which is computationally demanding. The difference between the approximate solution of REML and the exact solution could be narrowed by magnifying the diagonal elements. One can take

Table 2. Approximate estimates of the trace, u′u and u′Z′MY for different ratio ($R = \propto I$) and different sets of matrices.

$\propto$	Set	Trace	u′u	u′Z′MY
	DI	.32979	72.166	1480.590
	First	.32499	80.036	1558.700
15	Second	.32899	76.763	1525.140
	Third	.32782	80.533	1563.790
	DI	.11232	9.854	548.000
	First	.11213	10.227	558.282
50	Second	.11229	10.070	553.923
	Third	.11222	10.385	562.415
	DI	.1192	.11925	60.299
	First	.01192	.11974	60.456
500	Second	.01192	.11953	60.367
	Third	.01192	.12001	48.903

DI = direct inversion, First Set = $(Z'MZ)$, $(Z'MZ)$, (Z'_1MZ_1), Second Set = $(Z'MZ+\propto I)$, $(Z'_1MZ_1+\propto I)$, Third set = $(Z'MZ+\propto I)$,$(Z'MZ+\propto A^{-1})$

Table 3. Approximate estimates of the trace, u′u and u′Z′MY for different ratio ($R = \propto A^{-1}$) and different sets of matrices.

$\propto$	Set	Trace	u′u	u′Z′MY
	DI	.35166	75.392	1808.720
	First	.35121	81.569	1540.660
15	Second	.35121	78.075	1506.120
	Third	.38007	147.574	1624.480
	DI	.11459	12.460	738.140
	First	.11455	9.999	550.488
50	Second	.11457	9.838	546.014
	Third	.12845	32.043	737.552
	DI	.01194	.16871	85.931
	First	.01194	.11925	60.301
500	Second	.01194	.11903	60.240
	Third	.01366	.43684	85.994

DI = direct inversion, First Set = $(Z'MZ)$, (Z'_1MZ_1), Second Set = $(Z'MZ+\propto I)$, $(Z'_1MZ_1+\propto I)$, Third set = $(Z'MZ+\propto I)$,$(Z'MZ+\propto A^{-1})$

advantage of the large diagonal elements relative to small off-diagonal elements and diagonalize mixed model coefficient matrices after adding to diagonal element. Flury and Gautschi [6] found that iterative F-G algorithm converges faster with large diagonal elements. Moreover, Schaeffer [11] found that the iterative solution of large mixed model converges faster with large diagonal elements, and the larger are the diagonals compared to off-diagonal elements in the equations, the faster will be the rate of convergence.

Two criteria must be met to achieve complete diagonality and consequently finding an exact solution:
1) the diagonal elements of the transformed matrices are identical with their respective eigenvalues. Comparison of diagonal elements and their corresponding eigenvalues in the numerical example was given in Table 4 and 5. Diagonal elements and the eigenvalues became close to each other as increased to 500. The agreement of diagonal elements with the corresponding eigenvalues needs to be checked using likelihood ratio test as suggested by [10]. If the diagonal elements and their corresponding eigenvalues differ significantly then approximate estimation should be considered cautiously.

2) $Q(B) = 1$ where

$$Q(B) = \frac{|\,\mathrm{Diag}\,(B'C_iB)\,|}{|\,C_i\,|}$$

$|(\mathrm{diag}(B'C_iB))|$ = the product of all diagonal elements of the matrix inside the parenthesis.

$Q(B)>1$ if the off-diagonal elements deviate from zero. Table 6 shows estimates of $Q(B)$ for different sets of simultaneous transformation. As $\propto$ increased to 500, $Q(B)$ become close to 1. Diagonalizing $Z'MZ$ and $Z'_1\,MZ_1$ gave large values of $Q(B)$, and this is mainly due to the very small determinant of both matrices, $\det(Z'MZ)=2.5941E\text{-}13$, and $\det(Z'_1MZ_1)=-2.1110E\text{-}15$.

Flury and Gautschi [6] showed that two minima of equation (1) are expected if the matrix has small determinant, i.e. if the essentricity ($\frac{\mu_{max}}{\mu_{min}}$, where u is the eigenvalue) is high.

One can easily find that sums of squares of the off-diagonals for coefficient matrices are less after applying F-G and mf-G algorithms. Moreover, in terms of abso-

Table 4. Diagonal elements (DE) and eigenvalues (EV) for different sets of coefficient matrices and for different ratio

	R = 15 I		R = 50 I		R = 500 I	
Set-1	DE	EV	DE	EV	DE	EV
	20.738	22.016	55.738	57.016	505.738	507.016
	17.841	17.916	52.841	52.916	502.841	502.916
First	19.388	20.844	54.388	55.855	504.388	505.843
	18.298	17.916	53.298	54.358	503.298	504.358
	17.499	16.067	52.499	52.370	502.499	501.067
	17.437	15.000	52.437	50.000	502.437	500.000
	21.017	22.016	56.002	57.012	505.973	507.052
	15.157	15.157	50.166	49.998	500.156	499.973
Second	21.269	20.842	56.267	55.843	605.325	505.842
	19.393	19.358	54.389	54.355	504.385	504.349
	16.112	16.067	51.110	51.063	501.091	501.039
	18.253	18.253	53.253	52.915	503.290	502.039
	20.489	21.666	55.302	57.014	505.141	507.007
	15.460	15.062	55.842	55.846	505.824	505.849
Third	16.674	16.008	54.652	54.362	504.643	504.369
	19.406	19.406	50.816	49.999	501.058	500.025
	21.054	21.100	51.723	51.067	501.744	501.065
	18.074	17.914	52.866	52.915	502.821	502.919

First Set = $(Z'MZ)$, (Z'_1MZ_1), Second Set = $(Z'MZ+\propto I)$, $(Z'_1+\propto I)$, $(Z'_1MZ_1+\propto I)$ Third Set = $(Z'MZ+\propto I)$, $(Z'MZ+\propto A^{-1})$.

Table 5. Diagonal elements (DE) and eigenvalues (EV) for different sets of coefficient matrices and for different ratio

	R = 15A-1		R = 50A-1		R = 500A-1	
Set	DE	EV	DE	EV	DE	EV
	24.590	24.625	59.599	59.625	509.590	509.625
	15.374	15.000	50.374	50.002	500.374	500.000
First	17.038	18.014	52.038	53.014	502.038	503.014
	16.061	16.009	51.061	51.009	501.061	501.009
	16.470	16.251	51.470	51.415	501.470	501.251
	15.783	15.415	50.783	50.415	500.783	500.415

Table 5. Diagonal elements (DE) and eigenvalues (EV) for different sets of coefficient matrices and for different ratio

Set	$R = 15A^{-1}$ DE	$R = 15A^{-1}$ EV	$R = 50A^{-1}$ DE	$R = 50A^{-1}$ EV	$R = 500A^{-1}$ DE	$R = 500A^{-1}$ EV
	24.542	24.623	59.552	59.622	509.538	509.600
	15.660	15.416	50.645	49.996	500.622	499.600
Second	18.010	18.014	53.006	53.010	503.061	503.068
	15.829	16.252	50.823	51.252	500.820	501.271
	15.581	14.998	50.581	50.414	500.562	500.383
	15.693	16.010	50.695	51.006	500.730	501.026
	20.360	20.318	55.202	55.202	505.130	505.130
	4.217	4.215	105.848	105.842	1005.760	1005.760
Third	91.000	91.032	289.898	289.899	2856.070	2856.070
	34.700	34.800	12.734	12.473	116.517	116.517
	32.046	31.944	101.731	101.731	1001.740	1001.740
	43.892	43.906	134.357	134.364	1317.420	1317.420

First Set = $(Z'MZ)$, (Z'_1MZ_1), Second Set = $(Z'MZ+I)$, $(Z'_1+\propto I)$, $(Z'_1MZ_1+\propto I)$ Third Set = $(Z'MZ+\propto I)$, $(Z'MZ+\propto A^{-1})$.

Table 6. Estimates of Q(B) for different sets of coefficient matrices and for different ratio

Set	$\propto$ **15**	**50**	**500**
First	very large	very large	very large
Second	1.011265	1.001335	1.000000
Third	1.017800	1.002850	1.000061

First Set = $(Z'MZ)$, (Z'_1MZ_1), Second Set = $(Z'MZ+\propto I)$, $(Z'_1MZ_1+\propto I)$, Third Set = $(Z'MZ+\propto I)$, $(Z'MZ+\propto A^{-1})$.

lute value each diagonal entry is larger than the sum of off-diagonal entries in that row i.e.

$$|a_{ii}| > \sum_{j=1}^{n} |a_{ij}| \text{ for } j=1,2, \ldots\ldots, n.$$

At King Saud University IBM computer, the CPU time is combined with output machine time, so it is difficult to define CPU time used by either algorithm for diagonalizing two (6*6) matrices. However, Flury and Constantine [7] diagonalized two (6*6) matrices on MV 20 computer for MF-G algorithm with CPU time .070 seconds this compared with .101 seconds required for MF-G algorithm.

Conclusion

F-G and MF-G algorithms give approximate estimates of variance component of REML. Both algorithms gave the same transformation matrix (B). Equal or unequal weights n_1, ... , n_k can be used to achieve convergence for both algorithms and minimize the deviation from diagonality. Close estimate to the exact solution can be obtained for traits with low heritability (i.e large $\propto$) such as reproduction and fitness. Saving in CPU time by using MF-G algorithm becomes more important as the number of sires, animals in animal model, and traits increases.

F-G algorithm Adopted from Flury and Gautschi [1]

Let $\Phi(B) = \Phi(B' C_1 B, \ldots\ldots, B' C_k B; n_1, \ldots\ldots, n_k)$, the F-G algorithm yields a converging sequence of orthogonal matrices $B^o, B^1, \ldots\ldots$ such that $\Phi(B^{f+1}) \leqslant \Phi(B^f)$. The algorithm proceeds as follow:

F algorithm

Step Fo Define $B = (b_1, \ldots\ldots, b_p) \in 0(P)$ as an initial apporoximation to the orthogonal matrix minimizing Φ, e.g. B <----I, put F<------0.

Step F_1: Put $B^{(f)}$ <-----B and f<-----f+1'

Step F_2: Repeat steps F_{21} to F_{24} for all pairs (l,j), $l \leqslant 1 \leqslant j < p$

Step $F_{2\text{-}1}$: put H_{p*2} <----- (b_1, bj) and

$$T_1 <\!\!---- \begin{bmatrix} H'_1 C_i b_1 & b'_1 C_i b_j \\ & \\ b'_j C_i b_1 & b'_j C_i b_j \end{bmatrix}$$

The T_i are p.d.s. and (i = 1, ..., k).

Step $F_{2\text{-}z}$: Perform the G algorithm on (T_1, ..., T_k) to get an

$$\text{orthogonal matrix } Q = \begin{bmatrix} \text{Cos} \propto & -\sin\propto \\ \sin\propto & \cos\propto \end{bmatrix}$$

Step $F_{2\text{-}3}$: Put $H^*(p^*2)=(b^*_1,b^*_j)$ <------ HQ (This is an orthogonal rotation of the two columns of H by an angle $\propto$).

Step $F_{2\text{-}4}$: In the matrix B, replace columns b_1 and b_j by b^*_1 and b^*_j, respectively and call the new matrix again B.

Step F_3: If for some $\underset{p}{\epsilon}>0,\Phi(B^{f-1)}\text{-}\Phi<Bf) > \epsilon$ holds stop. Otherwise start the next iteration stop at F_1.

G-algorithm

This algorithm solves the equation:

$$q_1 \left[\sum_{i=1}^{k} n_i \frac{k_{i1} - k_{i2}}{k_{i1}\, k_{i2}} T_i \right] q_2 = 0, \text{ where} \tag{1}$$

$T_1,\ldots\ldots,T_k$ are fixed p.d.s. 2*2 matrices, $n_i>0$ are fixed constants, $k_{ij} = q'jTiqj$ (i = 1,......,k), j=1,2) and $Q = (q_1,q_2)$ is an orthogonal 2*2 matrix. The iteration of the sequence of orthogonal matrices $Q^o,Q^1,\ldots\ldots$, converging to a solution of the algorithm proceeds as follows:

Step Go: Define Q(2*2) as an initial approximation to the solution on (1).

$$Q <\text{--------} I_2 \qquad \text{put } g<\text{--------}0$$

Step G_1: Put Q(g)<-------Q and g<-------g+1

Step G_2: Compute k_{ij} using the algorithm

$$\sum_{i=1}^{k} n_i \frac{k_{i1} - k_{ij}}{k_{i1}k_{ij}} T_i$$

Step G3: Compute normalized eigenvectors of T. In $Q = (q_1, q_2)$, Put q_1 <------ first eigenvector of T, q_2 <------ second eigenvector of T.

Step G4: If $\| Q^{q-1} - Q \| < \epsilon$ stop. Otherwise start the next iteration step.

MF-G algorithm adopted from Clarkson [2]

1. Compute initial matrices $Q_I = B'_o C_i B_o$ (B_o matrix of initial estimates.

2. For column vectors (b_1, b_j) of B take the elements of T_1 as the corresponding diagonal and off-diagonal elements of Q_i. In other words $t_{i11} = q_{ijj}$, $t_{i22} = q_{i11}$, $t_{i12} = q_{iji}$ and $t_{i21} = q_{ij1}$

3. Update each matrix Q_i from the values c and s computed during the G step as

$$q^n_{ijj=c2}\, t_{i11} + 2csti_{12} + s^2 ti_{22}$$
$$q^2_{i11} = s^2 t_{i11} - 2cst_{i12} + c^2 t_{i22}$$
$$q^n_{ij1} = cs\,(t_{i22} - t_{i11}) + (c^2\, s^2)\, t_{i12}$$
$$q^n_{ij1} = qij1$$
$$q^n_{iml} = sq_{iml} + sq_{imj}$$
$$q^n_{iml} = sq_{iml} + sq_{imj}$$
$$q^n{imj} = q_{imj}$$
$$q^n_{i1m} = q_{im1}$$
where m = 1,……, p,m=1,m=j

4. Update the vectors (b_j, b_1) as discussed above using tangent.

5. Go to step 2 with a new pair (j,1) of indices for vectors (b_j, b_1).

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تطبيق طريقة حساب ف. ج الوترية على أعلى إمكانية محدودة لتقدير مكونات التباين

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ملخص البحث. يمكن استخدام طريقة حساب ف. ج للعالم فالوري وجاوتش (١٩٨٤م) لحساب المصفوفة ب التي تعطي أقل قيمة ممكنة للمعادلة

$$\text{ك}(\text{ب}) = \left(\frac{\text{محدد المصفوفة الوترية ب ج}_{\text{ر}}\text{ ب}}{\text{محدد المصفوفة ج}}\right)^{\text{ن}_{\text{ر}}}$$

حيث إن المصفوفة ج تكون في صورة رَ م ر + هـ أ$^{-1}$

وأن ن ر هي أوزان موجبة وأن رَ هو معكوس المصفوفة ر

أ$^{-1}$ هو مقلوب المصفوفة أ (مصفوفة القرابة)

$$\text{هـ} = \frac{\text{ت}_{\text{ر}}^{2}}{\text{ت}_{\text{س}}^{2}} = \frac{\text{تباين الانحراف البيئي}}{\text{التباين الوراثي للطلائق}}$$

المصفوفة ب تحول المصفوفات ج$_1$، ج$_2$، .... ج$_{\text{ق}}$ إلى مصفوفات قريبة من الوترية وبالتالي يمكن إيجاد مقلوب المصفوفة رَ م ر + هـ أ$^{-1}$. ولتقليل عدد دورات الحساب تمكن كالركسون (١٩٨٨م) باستخدام طريقة الحساب المعدلة م ف. ج لإيجاد المصفوفة ب والتي بوساطتها يمكن تحويل المصفوفة ج ر إلى مصفوفة قريبة من الوترية.

أمكن تطبيق طريقتي الحساب ف. ج، م ف. ج على ثلاث مجموعات من المعادلات المزدوجة والتي تستخدم كثيرًا في مجال تربية الحيوان وكان الحل في كل من طريقتي الحساب قريبًا من الطريقة المضبوطة عنـدما كان العمق الوراثي للصفة منخفضًا. وأمكن الحصول على النتائج نفسها عندما كانت الأوزان متساوية أو غير متساوية.