

Restricted Maximum Likelihood Procedures for the Estimation of Additive and Nonadditive Genetic Variances and Covariances in Multibreed Populations¹

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ABSTRACT: Restricted maximum-likelihood procedures were developed to estimate additive and nonadditive genetic and environmental covariances for multiple traits in multibreed populations. The computational procedure follows the expectation-maximization (EM) algorithm, where the set of equations in the maximization step is solved by successive approximations. This computational procedure does not guarantee convergence to a symmetric positive-definite covariance matrix. Thus, computer programs will need to incorporate restrictions in the maximization step to ensure positive definiteness of each covariance matrix. Additive genetic and environmental covariances were modeled in subclass form (zeros and ones in the design matrices). Nonadditive genetic covariances

were modeled in regression form (any value between and including zero and one in the design matrices). Computational requirements will be larger than for intrabreed analyses. Appropriate simplifying assumptions and numerical techniques (e.g., sparse and iterative numerical techniques) will be required for the implementation of these multibreed covariance estimation procedures. Number of iterations (5 to 12) and computing times (57 to 113 min) to achieve convergence when estimating 21 genetic and environmental covariances in five small simulated multibreed data sets (two breeds, 25,200 to 50,400 calves, 120 to 135 unrelated bulls) suggest that these procedures are computationally feasible.

Key Words: Maximum Likelihood, Variance Components, Genetic Parameters, Population Structure

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Although crossbreeding is widely practiced in the United States, the active genetic basis of the beef industry is formed by a large number of breeds (e.g., Angus, Brahman, Hereford, Limousin, Simmental) that act independently of one another. Consequently, genetic evaluation and selection of parents are still formally carried out within each breed, as evidenced by the Guidelines for Uniform Beef Improvement Programs (BIF, 1990). Unfortunately, intrabreed EPD cannot be used to compare bulls of the same or different breeds for crossbreeding purposes because they consider only additive genetic effects (each breed has a different additive genetic base) and they ignore nonadditive genetic effects (defined here as the combining ability of a bull when mated to dams of various breed compositions). If bulls are to be compared across breeds and crossbred groups both

additive and nonadditive genetic effects will need to be accounted for (Elzo and Famula, 1985). In a multibreed genetic evaluation, each breed and crossbred group may have different values for additive genetic variances and covariances (Elzo, 1990a; Lo et al., 1994). Similarly, each breed group combination may have different values for nonadditive genetic variances and covariances (Elzo, 1990b). Environmental variances and covariances may also differ across breeds and crossbred groups. The large number of sets of additive, nonadditive, and environmental covariances that need to be estimated simultaneously can be drastically reduced if multibreed covariances are assumed to be linear functions of a small set of covariances.

The current method of choice to estimate covariances using animal breeding data is REML. However, existing REML procedures can only estimate a single set of covariances. Thus, the objective of this research was to develop REML procedures for multibreed populations that 1) account for heterogeneity of covariances across genetic groups of animals, 2) express additive and nonadditive genetic and environmental covariances of genetic groups as linear combinations of a small number of covariances, and 3) simultaneously estimate all the sets of covariances

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used to compute all the additive and nonadditive genetic and environmental covariances of any genetic group given a set of base breeds.

Development of the Restricted Maximum Likelihood Procedure to Estimate Covariances in Multibreed Populations

The computational procedure is based on the expectation-maximization (EM) algorithm (Dempster et al., 1977), where the maximization step is accomplished by iteration.

The description of this procedure requires the use of unfamiliar terminology as well as definitions of multibreed additive, nonadditive, environmental, and residual covariances. Thus, these preliminary aspects will be explained first.

Definition of Terms

Multibreed population: a population composed of straightbred and crossbred animals.

Breed group: a group of animals whose genetic composition falls within a range of fractions of breeds; for example, if five breed groups are constructed to group animals in a two-breed population (A = breed 1, B = breed 2), the group ranges could be as follows: group 1 = (.10 to .81)A (.0 to .19)B, group 2 = (.80 to .61)A (.20 to .39)B, group 3 = (.60 to .41)A (.40 to .59)B, group 4 = (.40 to .21)A (.60 to .79)B, and group 5 = (.0 to .19)A (.10 to .81)B.

Regression model: a model that defines multibreed bull nonadditive effects in terms of intra- and interbreed interactions between alleles at l loci, $l = 1, \dots, L$.

Bull model: an abbreviation of sire-maternal grand-sire model.

Additive intrabreed genetic covariance: a covariance due to additive genetic effects within a breed.

Additive interbreed genetic covariance: a covariance arising from differences between intrabreed means of additive genetic effects; it is equal to twice the segregation covariance (Lo et al., 1994).

Additive multibreed genetic covariance: an additive covariance for animals in a multibreed population; equal to either an additive intrabreed genetic covariance (straightbred animals) or a weighted sum of additive intrabreed and interbreed genetic covariances (progeny of at least one crossbred parent).

Nonadditive configuration: a representation of l loci using the breed of origin of the alleles. For two breeds, A and B, there are four configurations at one locus: A/A, A/B, B/A, and B/B; three configurations result if A/B and B/A are defined as one configuration. A possible set of configurations for one and two loci is shown in Elzo (1990b).

Nonadditive intraconfiguration genetic covariance: a covariance due to nonadditive genetic effects caused by the interaction between alleles of one or

more breeds within a nonadditive configuration. Nonadditive configurations are to nonadditive genetic covariances as breeds are to additive genetic covariances.

Environmental intrabreed genetic covariance: a covariance due to environmental effects within a breed.

Environmental interbreed genetic covariance: a covariance arising from differences between intrabreed means of environmental effects.

Environmental multibreed genetic covariance: an environmental covariance equal to either an intrabreed environmental covariance (straightbred animals) or a weighted sum of intrabreed and interbreed environmental covariances (progeny of one or two crossbred parents).

Residual intrabreed, interbreed, and multibreed genetic covariances: weighted sums of additive and environmental intrabreed, interbreed, and multibreed covariances.

Assumptions

The following assumptions are made: 1) traits are determined by a large number of unlinked loci, 2) random segregation and assortment of alleles occur during meiosis, 3) no inbreeding, and 4) covariances remain constant over time.

Additive Multibreed Genetic Covariances

Additive genetic covariances for each breed group combination are assumed to be different. These covariances are equal to the sum of two terms. The first term is equal to the weighted sum of the intrabreed covariances for traits Y and Z, where the weights are the expected frequencies of each breed in the g^{th} breed group combination (Elzo, 1983, 1990a; Lo et al., 1994). The second term is equal to the weighted sum of the interbreed covariances for traits Y and Z, where the weights are the sum of the product of the expected breed frequencies in the parental breed groups (Lo et al., 1994). This second term was assumed to be zero by Elzo (1990a). Inclusion of the second term in the computation of multibreed additive covariances does not affect the rules to compute the matrix of covariances among bull additive genetic effects (G_a) or its inverse (G_a^{-1}).

Thus, the additive genetic covariance between traits Y and Z for an animal in a noninbred multibreed population is

$$\text{cov}_a(Y, Z) = \sum_{b=1}^{nb} p_b^i (\sigma_{aYZ})_b + \sum_{b=1}^{nb-1} \sum_{b'>b}^{nb} (p_b^s p_{b'}^s + p_b^d p_{b'}^d) (\sigma_{aYZ})_{bb'} \quad [1]$$

where the superscripts *i*, *s*, and *d* correspond to individual animal, sire, and dam, the subscripts *b* and *b'* represent two breeds, and *nb* = number of breeds; p_b^x = expected fraction of breed *b* in animal *x*, *x* = *i*, *s*, *d*; $(\sigma_{aYZ})_b$ = additive intrabreed covariance for breed *b*; and $(\sigma_{aYZ})_{bb'}$ = additive interbreed covariance for the pair of breeds *b* and *b'*.

Nonadditive Multibreed Genetic Covariances

Nonadditive genetic effects were accounted for by means of regression procedures. Thus, nonadditive intraconfiguration covariances between traits *Y* and *Z* at *l* loci, $(\sigma_{nYZ})_l$, *l* = 1, ... , *L*, need to be estimated. These covariances are not a function of any other set of nonadditive covariances. This characteristic makes nonadditive covariances in regression models different from additive genetic covariances, which are assumed to be a function of intra- and interbreed additive covariances.

Environmental and Residual Multibreed Covariances

Multibreed environmental covariances could be assumed 1) to be equal for all breeds and crossbred groups, 2) to be different for each breed and crossbred group (i.e., given an environment each genotype reacts differently), and 3) something in between alternatives 1 and 2.

If multibreed environmental covariances were assumed 1) to be different across breed groups, and 2) to behave in an additive fashion, then their computation would be similar to the procedure used to compute additive genetic covariances. Thus, the multibreed environmental covariance between traits *Y* and *Z* would be

$$\text{cov}_e(Y,Z) = \sum_{b=1}^{nb} p_b^i (\sigma_{eYZ})_b + \sum_{b=1}^{nb-1} \sum_{b'>b}^{nb} (p_b^s p_{b'}^s + p_b^d p_{b'}^d) (\sigma_{eYZ})_{bb'} \quad [2]$$

where the superscript *i* represents an individual animal, the subscripts *b* and *b'* represent two breeds, $(\sigma_{eYZ})_b$ = environmental intrabreed covariance for breed *b*, and $(\sigma_{eYZ})_{bb'}$ = environmental interbreed covariance for the pair of breeds *b* and *b'*.

The structure of the residual covariances will depend on 1) the additive model used (animal, reduced animal, sire-dam, bull, sire model), 2) the ancestors identified on an animal with records, and 3) the assumptions made with respect to multibreed environmental covariances.

An expression for the multibreed residual covariance between traits *Y* and *Z* for a bull model is the following:

$$\text{cov}_v(Y,Z) = \text{cov}_a(Y,Z)^i - \delta^s .25\text{cov}_a(Y,Z)^s - \delta^{mgs} .0625 \text{cov}_a(Y,Z)^{mgs} + \text{cov}_e(Y,Z)^i \quad [3]$$

where the superscripts *i*, *s*, and *mgs* refer to an animal, its sire, and its maternal grandsire, the subscripts *v*, *a*, and *e* represent residual, additive genetic, and environmental, and δ^x = indicator equal to 1 if animal *x* is not identified and to 0 if animal *x* is identified, *x* = *s*, *mgs*; $\text{cov}_a(Y,Z)^i = \text{cov}_a(Y_D,Z_D)^i$, where the subscript *D* = direct genetic effects; $\text{cov}_a(Y,Z)^s = \text{cov}_a(Y_D,Z_D)^s$; and $\text{cov}_a(Y,Z)^{mgs} = \text{cov}_a(Y_D,Z_D)^{mgs}$.

Additive genetic covariances in Equation [3] are computed using Equation [1] and environmental covariances using Equation [2]. If a model includes sires and dams, then additive dam covariances (and multiplying factors δ^d and .25) will be substituted for those of the maternal grandsire.

Model

Let a bull model be

$$y = Xb + Zu + v$$

$$\begin{bmatrix} y \\ u \\ v \end{bmatrix} \sim \text{MVN} \left\{ \begin{bmatrix} X\beta \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} ZGZ' + R ZG R \\ GZ' & G & 0 \\ R & 0 & R \end{bmatrix} \right\} \quad [4]$$

where *y* = vector of observations on all traits recorded per calf; *b* = vector of fixed effects for the *nt* traits being considered; *u* = vector of additive and nonadditive bull genetic effects for *nt* traits; *v* = vector of residuals; *X* = incidence matrix relating records to elements of *b*; *Z* = incidence matrix relating records to elements of *u*; *G* = matrix of covariances among elements of *u*; and *R* = matrix of covariances among elements of *v*.

Bulls are assumed to be unrelated. Bull genetic effects due to different nonadditive configurations are assumed to be uncorrelated among themselves and to additive genetic effects. Thus, the matrix *G* is block diagonal (one block per bull), with blocks

$$\begin{bmatrix} G_{0sg} & 0 & 0 & \dots & 0 \\ 0 & G_{0n1} & 0 & \dots & 0 \\ 0 & 0 & G_{0n2} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & G_{0nK} \end{bmatrix}$$

[5]

where

G_{0ag} = $nt \times nt$ matrix of additive direct genetic covariances for bulls of parental breed combination g , $g = 1, \dots, nbgcom$, where $nbgcom$ = number of different breed group combinations ($nbg(nbg + 1)/2$, nbg = number of breed groups); covariances in G_{0ag} are computed using Equation [1];

G_{0nk} = $nt \times nt$ matrix of nonadditive direct genetic covariances; $k = 1, \dots, K$, where $K = \sum_{l=1}^L nl$, and nl = number of interaction effects at l loci.

Calves are assumed to be related only through their sires and(or) maternal grandsires. Thus, residual effects are correlated only within a calf. Consequently, the matrix R is block diagonal, with blocks equal to R_{0m}^* , for $m = 1, \dots, M$, and M = number of residual subclasses (defined according to the various intra- and interbreed genetic and environmental factors contained in them). The R_{0m}^* are $nt \times nt$ matrices of residual covariances with zeros in the rows and columns corresponding to missing traits in a calf. Elements of R_{0m}^* are computed using Equation [3].

To simplify the notation, let $\phi = [\phi_a \ \phi_n \ \phi_e]'$ where ϕ_a is a vector of additive genetic covariances (the σ_{aYZ} in Equation [1]), ϕ_n is a vector of nonadditive genetic covariances (the $(\sigma_{nYZ})_l$), and ϕ_e is a vector of environmental covariances (the σ_{eYZ} in Equation [2]). Also, let the number of 1) additive genetic covariances be N_a , 2) nonadditive genetic covariances be N_n , 3) environmental covariances be N_e , and 4) $N_c = N_a + N_n + N_e$. Thus, each covariance in G_{0ag} , G_{0nk} , and R_{0m}^* is a linear function of elements of ϕ .

Computational Procedure

The derivation of the computational procedure used to obtain REML estimates of covariances (ϕ) in multibreed populations is described in the Appendix. The computational procedure makes use of the Expectation Maximization (EM) algorithm (Dempster et al., 1977). The EM algorithm is an iterative procedure that has an expectation step (**E-step**) and a maximization step (**M-step**) in each iteration. The E-step requires the computation of sums of products of predicted values of random effects plus their corresponding error variances of predictions (**EVP**). In the M-step, $\phi^{(p+1)}$ is computed by iteration, where $\phi^{(p)}$ is the value of ϕ that maximizes $Q(\phi | \phi^{(p)})$ (Equation [3], Appendix). Thus, at convergence, the M-step produces the covariance estimates for the $(p+1)^{th}$ EM iteration. The M-step is accomplished by iteration because the differentiation of $Q(\phi | \phi^{(p)})$ with respect to ϕ results in a nonlinear set of equations. The computing algorithm is as follows:

- Step 0.** 1) Define a set of initial covariance values.
2) Compute the matrices of derivatives of additive, nonadditive, and residual covariance matrices with respect to ϕ .
- E-Step.** 1) Compute the additive and nonadditive genetic and environmental sets of multibreed covariance matrices needed in the construction of the MME of the bull model.
2) Compute the predicted values of u_a and u_n (by solving the MME of the bull model) and v (by Equation [7], Appendix). Also, compute the EVP of u_a and u_n (using elements of the inverse of the MME) and v (by Equation [8], Appendix).
3) Compute $S_{0ag}^{(p)}$ (Equation [4], Appendix), $S_{0nk}^{(p)}$ (Equation [5], Appendix), and $S_{0m}^{(p)}$ (Equation [6], Appendix).
- M-Step.** 1) Compute $\phi^{(p+1)}$ by successive approximations (i.e., Scoring iterations) using Equations [12] (Appendix). If the difference between the absolute values of the estimates of $\phi^{(p+1)}$ and $\phi^{(p)}$ are less than or equal to a vector of small values ϵ (Equations [13] and [14], Appendix), then stop; otherwise, go back to the E-step and continue with the EM iterations.

Analyses of Simulated Data Sets

Five data sets were simulated and covariance components estimated using the methodology presented here. The purpose of these analyses was to obtain some information on the computer times and the number of EM and Scoring iterations required to achieve convergence in small data sets. Computations were carried out in an IBM RS6000 workstation, model 580, using a computer program (written in FORTRAN and compiled using the AIX XL FORTRAN Compiler/6000 without any optimization) based on the procedures described here. This program used the FSPAK sparse-matrix routines (Perez-Enciso and Misztal, personal communication) to invert the left-hand side of the MME.

Simulation of Data

Two breeds (A and B), two traits per calf, and only direct genetic effects were considered. Three additive genetic effects, one nonadditive genetic effect, three environmental effects and two sex effects were used in the simulation of calf records. All effects, except sex of calf, were simulated as random effects. The additive genetic effects were additive intrabreed A, additive intrabreed B, and additive interbreed AB. The nonadditive genetic effect was intraconfiguration 11 (one A allele and one B allele at one locus). Environmental effects were intrabreed A, intrabreed B, and interbreed AB. Sex effects were male and female.

Five breed groups in 20% intervals were defined. Between 120 and 135 unrelated bulls were generated by mating individuals of these five breed groups (15 breed group combinations). Progeny (between 25,200 and 50,400) were generated by mating these bulls to dams of all 15 breed-group combinations. There were between eight and nine bulls for each one of the 15 breed-group combinations. Maternal grandsires were chosen at random among the generated bulls (except for the avoidance of inbreeding).

The first line of each covariance in Table 1 is the values of the priors of the covariance matrices used to simulate calf records. Although no trait names are needed, Trait 1 could represent birth weight and Trait 2 weaning weight; thus, numbers in Table 1 would be in squared kilograms.

Estimation of Covariance Components

The simulated data were analyzed using a bull model that had sex as a fixed effect and sire and maternal grandsire additive as well as nonadditive genetic effects and residual effects as random effects. The vector of unknown covariances ϕ had 21 elements: three additive genetic covariances for breed A, three additive genetic covariances for breed B, three interbreed AB additive genetic covariances, three inter-

breed AB nonadditive genetic covariances, three environmental covariances for breed A, three environmental covariances for breed B, and three interbreed AB environmental covariances.

All genetic and environmental covariances for the two traits were estimated simultaneously. The convergence criterion used for the Scoring and the EM iterations was that the maximum absolute difference between two iterations had to be less than a preset small number. This number was .01 for both the Scoring and the EM iterations.

The only set of computations that is done only once in the computer program is the construction of 1) six intrabreed and three interbreed matrices of derivatives of additive genetic covariances for each one of the 15 breed-group combinations ($15 \times 9 = 135$ matrices), 2) one matrix of derivatives of nonadditive genetic covariances, and 3) six intrabreed and three interbreed matrices of derivatives of environmental covariances resulting from the mating of sires of 15 breed-group combinations to dams of 15 breed group combinations ($15 \times 15 \times 9 = 2,025$ matrices).

The computations carried out in every round of EM and Scoring iterations were as follows.

E-Step. Inverses of the matrices of covariances of bull additive and nonadditive genetic effects and environmental effects were computed. The number of

Table 1. Covariance priors, means, and range of values of REML estimates for two traits from five stimulated data sets

Covariance	Pairs of traits		
	(1,1)	(1,2)	(2,2)
Additive			
Intrabreed A	4.0 ^a	3.0	40.0
	3.8 ^b	2.7	40.8
Intrabreed B	(1.7, 5.7) ^c	(-6, 5.6)	(17.0, 55.0)
	6.0	4.0	60.0
Interbreed AB	6.2	5.2	52.4
	(3.9, 7.6)	(3.9, 6.8)	(41.7, 60.3)
Nonadditive (1 locus)	2.0	4.0	20.0
	1.9	1.8	27.0
Intraconfiguration 11	(1.2, 3.2)	(-3.3, 5.8)	(11.1, 48.7)
	3.0	4.0	30.0
Environmental	4.8	5.8	38.9
	(4.1, 5.3)	(5.0, 7.6)	(32.2, 53.1)
Intrabreed A	6.0	7.0	90.0
	6.2	7.0	87.1
Intrabreed B	(4.9, 7.6)	(5.7, 9.0)	(72.4, 109.8)
	14.0	10.0	240.0
Interbreed B	14.1	8.8	238.9
	(12.9, 15.6)	(7.5, 9.4)	(233.1, 249.3)
Intraconfiguration 12	4.0	8.0	60.0
	4.3	10.1	67.8
Environmental	(3.5, 4.7)	(7.5, 12.7)	(50.4, 85.0)

^aCovariance prior.

^bMean of five REML estimates.

^c(Smallest, largest) value among five REML estimates.

matrices computed were 1) 15 additive genetic (one for each breed-group combination), 2) one nonadditive interbreed, and 3) 225 residual (one for each sire breed-group combination \times dam breed-group combination subclass). These matrices were used in the E- and M-steps of this procedure.

The predicted values of the vectors \mathbf{u}_a and \mathbf{u}_n and the matrices of their EVP were computed for all bulls. Also, the predicted values of the \mathbf{v} vectors and the matrix of their EVP were computed for all calves. These vectors and matrices were then used to compute matrices containing the sums of products of predicted values plus their EVP. The number of these matrices were 1) 15 matrices for bull additive genetic effects ($\mathbf{S}_{0ag}^{(p)}$, $ag = 1, \dots, 15$, Equation [4], Appendix), 2) one matrix for bull nonadditive genetic effects as regressors ($\mathbf{S}_{0n1}^{(p)}$, Equation [5], Appendix), and 3) 225 matrices for residual effects ($\mathbf{S}_{0m}^{(p)}$, Equation [6], Appendix).

M-Step. Matrices \mathbf{B}_{aa} , \mathbf{B}_{ae} , \mathbf{B}_{nn} , and \mathbf{B}_{ee} , and vectors \mathbf{d}_a , \mathbf{d}_n , and \mathbf{d}_e were computed here. These are the submatrices and subvectors of system of Equations [12] (Appendix). Matrices \mathbf{B}_{aa} , \mathbf{B}_{ae} , and \mathbf{B}_{ee} were (9×9). Matrix \mathbf{B}_{nn} was 3×3 . Vector \mathbf{d}_a was 9×1 , \mathbf{d}_n was 3×1 , and \mathbf{d}_e was 9×1 . The estimate of ϕ for the $(p+1)^{\text{th}}$ EM iteration was obtained by solving the resulting system of equations by successive approximations. Within each Scoring iteration, Equations [12] (Appendix) were solved by direct inversion of the $\{\mathbf{B}_{ij}\}$ matrix and subsequent multiplication by vector $\{\mathbf{d}_i\}$. The number of Scoring iterations to achieve convergence ranged between one and five.

Starting values were those of the covariances used to simulate the data set. These were 1) the nine additive genetic covariances (intra-breed A, intra-breed B, and interbreed AB), 2) the three covariances for nonadditive intra-configuration 11, and 3) the nine environmental covariances (intra-breed A, intra-breed B, and interbreed AB). It took from 8 to 12 EM iterations and between 57 min and 113 min to reach convergence.

The mean and the (smallest, largest) values of the REML estimates of covariances in ϕ of the five simulated samples are shown in lines two and three of each covariance in Table 1. The means indicate that in these few small data sets seven covariances were underestimated, two were equal to the parameter values, and 12 were overestimated. The smallest and the largest values of the covariance estimates as a percentage of the parameter values were 7.8 and 143.5%. The average absolute difference as a percentage of the parameter values was 17%.

Discussion

The REML methodology presented here will be useful not only in multibreed populations in which breeding animals are both straightbred and crossbred but also when straightbred animals are mated to

animals of other breed groups (straightbred or crossbred). In general, multibreed procedures can be applied whenever animals from several distinct subpopulations interbreed.

Modeling Aspects

The model used to present these procedures used a subclass approach to additive genetic effects, whereas a regression approach was used to account for nonadditive genetic effects. Another alternative could have been to use a regression approach to explain additive genetic effects. In the case of multibreed populations of two breeds, each bull would have up to two predicted additive genetic values: one due to its alleles from breed A and another from alleles of breed B. A third one could also be predicted for additive interbreed AB genetic effects. The matrix \mathbf{Z} for additive genetic effects will have up to three values per bull (between 0 and 1). The Equation for $Q_a(\phi | \phi^{(p)})$ will be similar to the one given for nonadditive genetic covariances in regression models ($Q_n(\phi | \phi^{(p)})$, Equation [5], Appendix).

Residual covariances were explained in terms of their additive and environmental components. Another option would have been to define residual covariances as part of the ϕ vector. In this case 1) the contributions of the residual function to additive genetic covariances will be zero, and 2) the set of Equations [12] (Appendix) will become block diagonal. Because of the large number of different residual covariances possible per trait, simplifying assumptions would need to be made. Possible alternatives could be 1) calves from each breed-group combination would have a unique set of residual covariances, 2) calves from each breed group would have a different residual covariance matrix, 3) residual covariances could be treated as additive genetic covariances, where each covariance would be a linear function of intra-breed and interbreed residual covariances, and 4) a single set of residual covariances is used for all calves.

Although the presentation of this methodology made use of a sire-maternal grandsire model for direct effects only, 1) more complete models (sire-dam, reduced animal and animal) can be programmed with multibreed features, and 2) maternal effects can also be included in the model and in computer programs. Incorporation of additional animals to be evaluated in the model and of maternal effects will increase computing times substantially. In a bull model, the programming of direct and maternal genetic effects is considerably more complex than the programming of direct genetic effects alone; however, this should be simpler in the sire-dam and (reduced) animal models.

Computational Aspects

The analyses of the small simulated data presented here included only one source of nonadditive variation (intra-locus interbreed). However, real data will

probably contain additional sources of nonadditive variation (e.g., intralocus intrabreed). Ideally all sources of nonadditive variation should be accounted for in the model. However, assumptions relative to the number of loci considered for nonadditive genetic covariances will usually need to be made because of cost or computational feasibility. Furthermore, which nonadditive genetic effects will be able to be included in the mixed model used to predict the u 's and the v 's will largely depend on the dependencies and multicollinearity that exist among them. These two factors need to be closely monitored in unbalanced data sets because missing data can cause both confounding and multicollinearity. If this happened, further simplifying assumptions may be needed to analyze those data sets.

The numbers of bulls and progeny per bull in field data sets will probably be substantially larger than the eight or nine bulls considered in the simulated data sets. Thus, the values of the covariance estimates should be closer to the parameter values than the ones obtained here, assuming that all important genetic and environmental effects were accounted for in the model.

The computing times of the simulations were probably longer than needed because the computer program used was a research tool that has not been optimized for speed. In addition, the computer program had checks at various points in the computational procedure that must have added time to each round of iteration. However, placing the covariances used in the simulation as priors is likely to reduce the number of EM iterations needed to achieve convergence. A small test was conducted to check whether 1) the number of EM iterations needed to achieve convergence and 2) the convergence values would be the same when priors were equal to and different from the simulation covariances. Two additional small data sets of similar structure and size to the five previous data sets were generated. Three runs per data set were carried out. In the first run, simulation covariances were used as priors. In the second run, the prior values used were lower than the simulation covariances. In the third run, prior values higher than the simulation covariances were used. In runs two and three, only two prior covariance matrices were used, one for all genetic effects and another for all environmental effects. The only consequence of using these low and high priors was the need for one additional EM iteration to achieve convergence; all covariance estimates at convergence were the same.

Programming Aspects

Programming these procedures is more involved than intrabreed procedures. Because of the number of random genetic effects to be predicted per bull may be substantially larger than for a single breed, sparse-matrix procedures (e.g., FSPAK, Perez-Enciso and Misztal, personal communication) become a must if solutions are to be obtained directly. For very large

data sets (tens of thousands to millions of animals) iterative procedures will be needed to compute predictions of u 's and v 's as well as suitable approximations to the EVP of the u 's and v 's.

Implications

The procedures to estimate covariance components developed here make possible the prediction of additive and nonadditive genetic values of animals in multibreed populations, in systematic crossbreeding programs, semen importation and, in general, when animals of several distinct subpopulations interbreed. Although their computational requirements may be substantially larger than intrabreed covariance estimation procedures, the number of covariances to be estimated can be largely decreased by using an appropriate set of assumptions.

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Appendix

Derivation of the Computational Procedure to Estimate Covariance Components in Multibreed Populations

The computational procedure used to solve for the REML estimates of ϕ makes use of the expectation-maximization (EM) algorithm (Dempster et al., 1977). The EM algorithm used here is based on the general version described by Dempster et al. (1977), which relies on the function

$$Q(\phi'|\phi) = E[\ln f(\mathbf{x}|\phi')|\mathbf{z},\phi] \quad [1]$$

which is assumed to exist for all pairs (ϕ', ϕ) , where \mathbf{x} = complete data and \mathbf{z} = incomplete data. Also, $f(\mathbf{x},\phi)$ is assumed to be an increasing function almost everywhere.

The incomplete data used here are defined to be a linear combination of the vector of observations, $\mathbf{K}'\mathbf{y}$, where \mathbf{K}' is a matrix of contrasts such that $\mathbf{K}'\mathbf{X} = \mathbf{0}$. The complete data are considered to be the vectors of unknown random effects in the model (\mathbf{u} and \mathbf{v}). The log-likelihood of the complete data, L_c , is:

$$\begin{aligned} \ln [f(\mathbf{u}_a, \mathbf{u}_n, \mathbf{v}|\phi)] &= \text{constant} + \ln [f(\mathbf{u}_a|\phi)] \\ &+ \ln [f(\mathbf{u}_n|\phi)] + \ln [f(\mathbf{v}|\phi)], \end{aligned} \quad [2]$$

where

$$\ln [f(\mathbf{u}_a|\phi)] = -\frac{1}{2} \sum_{ag=1}^{nbgcom} \sum_{i=1}^{n_{ag}} [\ln |G_{0ag}| + \mathbf{u}_{agi}' G_{0ag}^{-1} \mathbf{u}_{agi}],$$

$$\ln [f(\mathbf{u}_n|\phi)] = -\frac{1}{2} \sum_{i=1}^{n_{bu}} [\ln |G_{0nk}| + \mathbf{u}_{nki}' G_{0nk}^{-1} \mathbf{u}_{nki}], \text{ and}$$

$$\ln [f(\mathbf{v}|\phi)] = -\frac{1}{2} \sum_{i=1}^M \sum_{i=1}^{n_m} [\ln |R_{0m}^*| + \mathbf{v}_{mi}' (R_{0m}^*)^{-1} \mathbf{v}_{mi}],$$

and \mathbf{u}_a = vector of bull additive genetic effects; \mathbf{u}_n = vector of bull nonadditive genetic effects; n_{ag} = number of bulls in breed group combination ag ; n_{bu} = total number of bulls; and n_m = number of calves in calf group m .

The EM algorithm is an iterative procedure that has two steps in each iteration: 1) an expectation step (E-step), and 2) a maximization step (M-step). The E-step consists of computing $Q(\phi|\phi^{(p)})$, and in the M-step, $\phi^{(p+1)}$ is computed, where $\phi^{(p+1)}$ is the value of ϕ that maximizes $Q(\phi|\phi^{(p)})$. The M-step is accomplished by iteration because the differentiation of $Q(\phi|\phi^{(p)})$ with respect to ϕ results in a nonlinear set of equations. The derivation of the E-step and the M-step for the $(p+1)^{th}$ iteration is described below.

E-step. The function $Q(\phi|\phi^{(p)})$, ignoring the constant term, is

$$Q(\phi|\phi^{(p)}) = Q_a(\phi|\phi^{(p)}) + Q_n(\phi|\phi^{(p)}) + Q_v(\phi|\phi^{(p)}). \quad [3]$$

The function for additive genetic covariances is

$$\begin{aligned} Q_a(\phi|\phi^{(p)}) &= E[\ln [f(\mathbf{u}_a|\phi)]|\mathbf{K}'\mathbf{y},\phi^{(p)}] \\ &= E\left[-\frac{1}{2} \sum_{ag=1}^{nbgcom} \sum_{i=1}^{n_{ag}} (\ln |G_{0ag}| + \mathbf{u}_{agi}' G_{0ag}^{-1} \mathbf{u}_{agi})|\mathbf{K}'\mathbf{y},\phi^{(p)}\right] \\ &= -\frac{1}{2} \sum_{ag=1}^{nbgcom} \left[n_{ag} \ln |G_{0ag}| + \text{tr} G_{0ag}^{-1} \sum_{i=1}^{n_{ag}} E[\mathbf{u}_{agi} \mathbf{u}_{agi}'|\mathbf{K}'\mathbf{y},\phi^{(p)}] \right] \\ &= -\frac{1}{2} \sum_{ag=1}^{nbgcom} \left[n_{ag} \ln |G_{0ag}| + \text{tr} G_{0ag}^{-1} \mathbf{S}_{0ag}^{(p)} \right], \end{aligned} \quad [4]$$

where

$$\begin{aligned} \mathbf{S}_{0ag\bullet}^{(p)} &= \sum_{i=1}^{n_{ag}} \mathbf{E}[\mathbf{u}_{agi}\mathbf{u}_{agi}' | \mathbf{K}'\mathbf{y}, \phi^{(p)}] \\ &= \sum_{i=1}^{n_{ag}} \left(\mathbf{E}[\mathbf{u}_{agi} | \mathbf{K}'\mathbf{y}, \phi^{(p)}] \mathbf{E}[\mathbf{u}_{agi}' | \mathbf{K}'\mathbf{y}, \phi^{(p)}] + \text{var}(\mathbf{u}_{agi} | \mathbf{K}'\mathbf{y}, \phi^{(p)}) \right) \\ &= \sum_{i=1}^{n_{ag}} \left(\hat{\mathbf{u}}_{agi} \hat{\mathbf{u}}_{agi}' + \text{var}(\hat{\mathbf{u}}_{agi} - \mathbf{u}_{agi}) \right), \end{aligned}$$

and where

$$\begin{aligned} \hat{\mathbf{u}}_{agi} &= \text{BLUP of } \mathbf{u}_{agi}, \text{ and} \\ \text{var}(\hat{\mathbf{u}}_{agi} - \mathbf{u}_{agi}) &= \text{EVP of } \hat{\mathbf{u}}_{agi}. \end{aligned}$$

Similarly, the function for nonadditive genetic covariances is

$$\begin{aligned} Q_n(\phi | \phi^{(p)}) &= \mathbf{E}[\ln [f(\mathbf{u}_n | \phi)] | \mathbf{K}'\mathbf{y}, \phi^{(p)}] \\ &= \mathbf{E} \left[-\frac{1}{2} \sum_{i=1}^{n_{bu}} (\ln | \mathbf{G}_{0nk} | + \mathbf{u}_{nki}' \mathbf{G}_{0nk}^{-1} \mathbf{u}_{nki}) | \mathbf{K}'\mathbf{y}, \phi^{(p)} \right] \\ &= -\frac{1}{2} n_{bu} \ln | \mathbf{G}_{0nk} | - \text{tr} \mathbf{G}_{0nk}^{-1} \mathbf{S}_{0nk\bullet}^{(p)}. \end{aligned} \tag{5}$$

where

$$\begin{aligned} \mathbf{S}_{0nk\bullet}^{(p)} &= \sum_{i=1}^{n_{bu}} \mathbf{E}[\mathbf{u}_{nki}\mathbf{u}_{nki}' | \mathbf{K}'\mathbf{y}, \phi^{(p)}] \\ &= \sum_{i=1}^{n_{bu}} \left(\hat{\mathbf{u}}_{nki} \hat{\mathbf{u}}_{nki}' + \text{var}(\hat{\mathbf{u}}_{nki} - \mathbf{u}_{nki}) \right), \end{aligned}$$

and where

$$\begin{aligned} \hat{\mathbf{u}}_{nki} &= \text{BLUP of } \mathbf{u}_{nki}, \text{ and} \\ \text{var}(\hat{\mathbf{u}}_{nki} - \mathbf{u}_{nki}) &= \text{EVP of } \hat{\mathbf{u}}_{nki}. \end{aligned}$$

Finally, the function for residual covariances is

$$\begin{aligned} Q_v(\phi | \phi^{(p)}) &= \mathbf{E}[\ln [f(\mathbf{v} | \phi)] | \mathbf{K}'\mathbf{y}, \phi^{(p)}] \\ &= \mathbf{E} \left[-\frac{1}{2} \sum_{m=1}^M \sum_{i=1}^{n_m} (\ln | \mathbf{R}_{0m}^* | + \mathbf{v}_{mi}' (\mathbf{R}_{0m}^*)^{-1} \mathbf{v}_{mi}) | \mathbf{K}'\mathbf{y}, \phi^{(p)} \right] \\ &= -\frac{1}{2} \sum_{m=1}^M \left(n_m \ln | \mathbf{R}_{0m}^* | + \text{tr}(\mathbf{R}_{0m}^*)^{-1} \mathbf{S}_{0m\bullet}^{(p)} \right), \end{aligned} \tag{6}$$

where

$$\begin{aligned} \mathbf{S}_{0m\bullet}^{(p)} &= \sum_{i=1}^{n_m} \mathbf{E}[\mathbf{v}_{mi}\mathbf{v}_{mi}' | \mathbf{K}'\mathbf{y}, \phi^{(p)}] \\ &= \sum_{i=1}^{n_m} \left(\hat{\mathbf{v}}_{mi} \hat{\mathbf{v}}_{mi}' + \text{var}(\hat{\mathbf{v}}_{mi} - \mathbf{v}_{mi}) \right), \end{aligned}$$

and where

$$\begin{aligned}\hat{\mathbf{v}}_{mi} &= \text{BLUP of } \mathbf{v}_{mi}, \text{ and} \\ \text{var}(\hat{\mathbf{v}}_{mi} - \mathbf{v}_{mi}) &= \text{EVP of } \hat{\mathbf{v}}_{mi}.\end{aligned}$$

The EM algorithm requires the function $Q(\phi | \phi^{(p)})$ to increase at each EM iteration. This is accomplished by choosing $\phi^{(p+1)}$ as the value that maximizes $Q(\phi | \phi^{(p)})$. However, to compute $\phi^{(p+1)}$ by maximizing $Q(\phi | \phi^{(p)})$ in the M-step, only $\mathbf{S}_{0ag}^{(p)}$, $\mathbf{S}_{0nk}^{(p)}$, and $\mathbf{S}_{0m}^{(p)}$ are needed (i.e., the complete $Q(\phi | \phi^{(p)})$ function does not need to be computed). Thus, the quantities that need to be computed in the E-step are $\mathbf{S}_{0ag}^{(p)}$, $\mathbf{S}_{0nk}^{(p)}$, and $\mathbf{S}_{0m}^{(p)}$, which are functions of the predicted values of \mathbf{u}_a , \mathbf{u}_n , and \mathbf{v} and their respective EVP. The predicted values of \mathbf{u}_a and \mathbf{u}_n are obtained by solving the mixed-model equations (MME) for the bull model (Equation [4] in the main text) and their EVP from elements of the inverse of the left-hand side. The predicted values of \mathbf{v} are computed as

$$\hat{\mathbf{v}} = \mathbf{y} - \mathbf{X}\mathbf{b}^\circ - \mathbf{Z}\hat{\mathbf{u}}, \quad [7]$$

and their EVP as

$$\text{var}(\hat{\mathbf{v}} - \mathbf{v}) = \mathbf{X}\mathbf{C}^{11}\mathbf{X}' + \mathbf{X}\mathbf{C}^{12}\mathbf{Z}' + \mathbf{Z}\mathbf{C}^{21}\mathbf{X}' + \mathbf{Z}\mathbf{C}^{22}\mathbf{Z}', \quad [8]$$

where the $\{\mathbf{C}^{ij}\}$ are submatrices of the inverse of the left-hand side of the MME for the bull model.

M-step. The vector $\phi^{(p+1)}$ is computed by maximizing the function $Q(\phi | \phi^{(p)})$. This requires differentiating $Q_a(\phi | \phi^{(p)})$, $Q_n(\phi | \phi^{(p)})$ and $Q_v(\phi | \phi^{(p)})$ with respect to ϕ and equating the resulting set of equations to zero.

The derivative of the additive genetic function is

$$\left\{ \frac{\partial Q_a(\phi | \phi^{(p)})}{\partial \phi_i} \right\} = \left\{ - \sum_{ag=1}^{nbgcom} \left[n_{ag} \text{tr} \mathbf{G}_{0ag}^{-1} \frac{\partial \mathbf{G}_{0ag}}{\partial \phi_i} \mathbf{G}_{0ag}^{-1} \frac{\partial \mathbf{G}_{0ag}}{\partial \phi_j} \right] \right\} \phi + \left\{ \sum_{ag=1}^{nbgcom} \left[\text{tr} \mathbf{G}_{0ag}^{-1} \frac{\partial \mathbf{G}_{0ag}}{\partial \phi_i} \mathbf{G}_{0ag}^{-1} \mathbf{S}_{ag}^{(p)} \right] \right\}, \quad [9]$$

where $\mathbf{G}_{0ag}^{-1} \mathbf{G}_{0ag}$, \mathbf{G}_{0ag} written as $\sum_{j=1}^{N_a} \frac{\partial \mathbf{G}_{0ag}}{\partial \phi_j} \phi_j$, was inserted in the first term.

A similar strategy is used to obtain the derivative of the nonadditive and residual functions. Thus, the derivative of the nonadditive genetic function is

$$\left\{ \frac{\partial Q_n(\phi | \phi^{(p)})}{\partial \phi_i} \right\} = \left\{ -n_{bu} \text{tr} \mathbf{G}_{0nk}^{-1} \frac{\partial \mathbf{G}_{0nk}}{\partial \phi_i} \mathbf{G}_{0nk}^{-1} \frac{\partial \mathbf{G}_{0nk}}{\partial \phi_j} \right\} \phi + \left\{ \text{tr} \mathbf{G}_{0nk}^{-1} \frac{\partial \mathbf{G}_{0nk}}{\partial \phi_i} \mathbf{G}_{0nk}^{-1} \mathbf{S}_{nk}^{(p)} \right\}, \quad [10]$$

and the derivative of the residual function is

$$\left\{ \frac{\partial Q_v(\phi | \phi^{(p)})}{\partial \phi_i} \right\} = \left\{ - \sum_{m=1}^M \left[n_m \text{tr}(\mathbf{R}_{0m}^*)^{-1} \frac{\partial \mathbf{R}_{0m}^*}{\partial \phi_i} (\mathbf{R}_{0m}^*)^{-1} \frac{\partial \mathbf{R}_{0m}^*}{\partial \phi_j} \right] \right\} \phi + \left\{ \sum_{m=1}^M \left[\text{tr}(\mathbf{R}_{0m}^*)^{-1} \frac{\partial \mathbf{R}_{0m}^*}{\partial \phi_i} (\mathbf{R}_{0m}^*)^{-1} \mathbf{S}_{0m}^{(p)} \right] \right\} \quad [11]$$

The set of equations to be solved in the M-step is

$$\begin{bmatrix} \mathbf{B}_{aa} & \mathbf{0} & \mathbf{B}_{aa} \\ \mathbf{0} & \mathbf{B}_{nn} & \mathbf{0} \\ \mathbf{B}_{aa} & \mathbf{0} & \mathbf{B}_{ee} \end{bmatrix} \begin{bmatrix} \phi_a \\ \phi_n \\ \phi_e \end{bmatrix} = \begin{bmatrix} \mathbf{d}_a \\ \mathbf{d}_n \\ \mathbf{d}_e \end{bmatrix}, \quad [12]$$

where

$$\mathbf{B}_{aa} = \left\{ \sum_{ag=1}^{nbgcom} n_{ag} (\text{tr} \mathbf{G}_{0ag}^{-1} \mathbf{D}_{0agi} \mathbf{G}_{0ag}^{-1} \mathbf{D}_{0agi}) + \sum_{m=1}^M n_m (\text{tr}(\mathbf{R}_{0m}^*)^{-1} \mathbf{D}_{0mi} (\mathbf{R}_{0m}^*)^{-1} \mathbf{D}_{0mj}^*) \right\},$$

and where

$$\mathbf{D}_{0agi} = \frac{\partial \mathbf{G}_{0ag}}{\partial \phi_i}, \mathbf{D}_{0mi} = \frac{\partial \mathbf{R}_{0m}^*}{\partial \phi_i}, \text{ and } i, j = 1, \dots, N_a;$$

$$\mathbf{B}_{ae} = \left\{ \sum_{m=1}^M n_m (\text{tr}(\mathbf{R}_{0m}^*)^{-1} \mathbf{D}_{0mi}^* (\mathbf{R}_{0m}^*)^{-1} \mathbf{D}_{0mj}^*) \right\} = \mathbf{B}_{ea}'$$

for $i = 1, \dots, N_a, j = N_a + N_n + 1, \dots, N_c$;

$$\mathbf{B}_{nn} = \left\{ n_{bu} (\text{tr} \mathbf{G}_{0nk}^{-1} \mathbf{D}_{0nki} \mathbf{G}_{0nk}^{-1} \mathbf{D}_{0nkj}) \right\},$$

and where

$$\mathbf{D}_{0nki} = \frac{\partial \mathbf{G}_{0nk}}{\partial \phi_i}, \text{ and } i, j = N_a + 1, \dots, N_a + N_n;$$

$$\mathbf{B}_{ee} = \left\{ \sum_{m=1}^M n_m (\text{tr}(\mathbf{R}_{0m}^*)^{-1} \mathbf{D}_{0mi}^* (\mathbf{R}_{0m}^*)^{-1} \mathbf{D}_{0mj}^*) \right\}, \text{ for } i, j = N_a + N_n + 1, \dots, N_c;$$

$$\mathbf{d}_a = \left\{ \sum_{ag=1}^{nbgcom} \text{tr} \mathbf{G}_{0ag}^{-1} \mathbf{D}_{0agi} \mathbf{G}_{0ag}^{-1} \mathbf{S}_{ag\bullet}^{(p)} + \sum_{m=1}^M \text{tr}(\mathbf{R}_{0m}^*)^{-1} \mathbf{D}_{0mi}^* (\mathbf{R}_{0m}^*)^{-1} \mathbf{S}_{m\bullet}^{(p)} \right\}, \text{ for } i = 1, \dots, N_a;$$

$$\mathbf{d}_n = \left\{ \text{tr} \mathbf{G}_{0nk}^{-1} \mathbf{D}_{0nki} \mathbf{G}_{0nk}^{-1} \mathbf{S}_{nk\bullet}^{(p)} \right\}, \text{ for } i = N_a + 1, \dots, N_a + N_n;$$

and

$$\mathbf{d}_e = \left\{ \sum_{m=1}^M \text{tr}(\mathbf{R}_{0m}^*)^{-1} \mathbf{D}_{0mi}^* (\mathbf{R}_{0m}^*)^{-1} \mathbf{S}_{m\bullet}^{(p)} \right\}, \text{ for } i = N_a + N_n + 1, \dots, N_c.$$

Equations [12]: 1) are nonlinear in ϕ , thus, $\phi^{(p+1)}$ must be computed iteratively (i.e., by successive approximations [Harville, 1977; Harville and Callahan, 1990]), 2) are equal to those obtained by a Scoring Algorithm applied to maximizing $Q(\phi | \phi^{(p)})$ (R. L. Quaas, Cornell University, personal communication), and 3) have no built-in restrictions on the values of the covariances, thus there is no guarantee that all parameters being estimated will be within the parameter space. Thus, computer programs need to incorporate restrictions to ensure that estimates of covariance matrices are symmetric positive definite (or at least symmetric positive semidefinite) at each Scoring iteration and at each EM iteration. Restriction strategies that could be considered include 1) barrier and penalty functions (Fletcher, 1974; Ryan, 1974; Harville, 1977), 2) gradient projection methods (Sargent, 1974; Harville, 1974), and 3) direct search methods (Swann, 1974).

The convergence criterion used to stop the Scoring and the EM iterations was that the absolute change in the estimates of covariances of two successive iterations was small (Bard, 1974; Searle et al., 1992). Thus, convergence was achieved when

$$|\phi^{(p+1)} - \phi^{(p)}| \leq \epsilon, \tag{13}$$

where ϵ is a vector of small numbers. The values of ϵ can be either set in advance or computed by the program (Bard, 1974). In the second case, Bard (1974) recommended using Marquardt's (1963) expression

$$\epsilon_i = \tau_1 (\phi_i^{(p)} + \tau_2). \tag{14}$$

where $\tau_1 = 10^{-4}$ and $\tau_2 = 10^{-3}$.