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Establishing bounds on the accuracies of predictions of breeding value

Paul Michael VanRaden

Iowa State University

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Establishing bounds on the accuracies of predictions of breeding value

by

Paul Michael VanRaden

A Thesis Submitted to the Graduate Faculty in Partial Fulfillment of the Requirements for the Degree of MASTER OF SCIENCE

Department: Animal Science
Major: Animal Breeding

Signatures have been redacted for privacy

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INTRODUCTION

Mixed model methodology has emerged as one of the most powerful tools available to animal breeders for the problems of parameter estimation and random variable prediction. Many genetic evaluations are routinely computed using mixed models with Best Linear Unbiased Prediction (BLUP) properties. Predictions obtained with BLUP have many desirable properties, and mixed model techniques seem appropriate for a wide range of statistical problems besides just those of animal breeders.

Because mixed model analyses such as sire evaluation sometimes involve very large systems of equations, methods to decrease the computation time required to obtain solutions have received much attention. This manuscript explores another such method to reduce computation time when working with large sets of mixed model equations. The method involves obtaining upper and lower bounds on prediction error variances and accuracies of solutions instead of exact answers through matrix inversion. Bounds are defined as expressions which lie on either side of some true value with probability equal to one. The method is demonstrated for only a simple cross-classified model, but these procedures may provide a general approach for dealing with more complex models. The bounds presented may also be useful for estimation of variance components.
REVIEW OF LITERATURE

Many of the problems which concern animals breeders are best described in terms of mixed linear models (Henderson, 1974). Mixed linear models are those in which the data vector is described as a linear function of fixed effects, random effects, and error. Over the last ten years, much research effort has been expended in an attempt to reduce the problem of mixed model estimation and prediction with large sets of data to a readily computable form.

Mixed models are a specific form of the more general Aitken system of equations (Henderson, 1974). In mixed models, certain random components are regarded as effects to be solved for rather than as part of the error structure. The Aitken equations require inverting the variance-covariance matrix V whose dimensions are equal to the number of observations in the data. Henderson's formulation of the mixed model avoids this problem by producing a system of equations with dimensions equal to the number of fixed plus random effects in the model.

In animal breeding applications, the technique of absorption is often used to further reduce the size of the system to be solved. With absorption, information contained in equations for one or more sets of effects is transferred to the remaining equations without ever explicitly solving for the effects being absorbed. In sire evaluation, for instance, herd-year-season equations are often absorbed to yield a system only as large as the number of sires or sires plus genetic
groups in the model. This may still result in a matrix too large to invert as national sire evaluations often involve several thousand sires.

A very useful technique to reduce computation costs in large systems is Gauss-Seidel iteration. This procedure avoids inversion of the coefficient matrix by obtaining successive approximations of the solution vector. The approximations are guaranteed to converge to the true solution for all positive definite matrices (Householder, 1964). Often, further improvements can be made to the Gauss-Seidel algorithm by including a relaxation factor and by adjusting the sire solutions to sum to zero after each iteration.

A rapid method for computing the inverse of a relationship matrix has been developed by Henderson (1975a) which allows for the inclusion of information from relatives with little additional computation cost. These techniques have enabled fairly sophisticated sire evaluation systems to be computed on a regular basis for many different traits. Examples are the Northeast A.I. Sire Comparison (Henderson, 1973) and the NAAB Calving Ease Summary (Freeman and Berger, 1981).

The most important output produced by these programs is usually the sire solutions which produce sire rankings. Often, however, other information is desired from the mixed model and this often requires much more effort in computing. Large matrix
inversion is not required for predicting sire merit, but is required for obtaining accuracies of predictions, prediction error variances, and estimates of variance components with the most desirable properties such as REML or MIVQUE. To avoid inversion, various attempts have been made to derive approximate formulae for accuracies or prediction error variances and to estimate variance components with procedures that have less than optimal properties. These formulae are necessary because of the expense, or even impossibility of getting inverses of very large systems of equations.

A common strategy has been to assume that the diagonal element of the inverse is approximately equal to the reciprocal of the original diagonal element before inversion. This is then multiplied by $\sigma_e^2$ to estimate prediction error variance (PEV). This procedure is used to calculate PEV in the NAAB Calving Ease Summary (Berger, P. J., 1983, personal communication, Iowa State University). Ufford et al. (1979) used a linear regression of the previous estimator to obtain a slightly better indicator of true PEV (computed by inversion). Ufford's study concluded that the estimator was very good for the specific data set considered. Another estimator listed by Ufford was one used in the Northeast A.I. Sire Comparison. It is simply a function of the number of daughters of the bull.

Recent studies not yet published by Weller et al. (1984) and Wilmink and Dommerholt (1984) have compared estimation of PEV by
the reciprocal of the diagonal element in models with and without relationships. Both concluded that this simple estimator performed well in models without relationships but that more sophisticated functions were needed for models with relationships included. Additionally, Weller attempted to estimate PEV in a multiple-trait model but had little success. In their conclusions, both Weller and Ufford stressed that estimation procedures developed in this manner lacked the generality to be applied to other models or even to other data sets.

Probably the most sophisticated formula used to report accuracy, called repeatability, is that used by USDA in the Modified Contemporary Comparison Sire Summaries (Dickinson et al., 1976). While USDA does not in fact use BLUP, its procedures based on selection index theory yield sire rankings similar to BLUP (Rothschild et al., 1976). Repeatability calculated in this approach is similar to $r_{IH}^2$ which was first used by Hazel (1943) to represent the squared correlation between predictor and predictand in a selection index context. Repeatability directly enters the formula for Predicted Difference (PD), being the regression factor multiplied by the daughters' difference from contemporaries. As will be seen later, a regression approach similar to repeatability will be used in deriving bound formulae in the mixed model.

Repeatability is a function of weights used to combine information from daughter records into the modified contemporary deviation. An
interesting aspect of these calculations is that the repeatability figure is arrived at iteratively, meaning that the repeatability of one bull is a function of the repeatabilities of bulls he is compared to (Norman, 1976). This leads one to speculate that an approach similar to Gauss-Seidel iteration might be used to obtain accuracy figures in mixed models without going through the process of large matrix inversion.

Numerous methods of variance component estimation have been proposed for and are in use by animal breeders. Henderson (1980) gave a brief review and comparison of many of these methods and in the same paper proposed a new method referred to as Henderson's Simple Method (HSM). Methods which have the most desirable properties such as minimum variance quadratic unbiased estimation (MIVQUE) or restricted maximum likelihood (REML) also have high computational costs. Two methods, MIVQUE(0) and HSM, which mimic the computations of MIVQUE, achieve great reductions in cost by assuming that off-diagonal elements of the coefficient matrix are trivially small compared to the diagonal elements. This allows the user to invert only diagonal matrices instead of full matrices.

Henderson (1980) stated that with regard to variance component estimation, "it is clear that animal breeders need a method for mixed models with large numbers of levels that is computationally feasible," but which still retains desirable properties. The ability to obtain bounds on diagonal elements of inverses without inversion would present a first step toward such a method.
METHODS

The model

Many of the models used by animal breeders and in fact all models that conform to the definition of mixed linear models may be represented by the equation

\[ y = Xb + Zu + e, \]

with definitions: \( y \) - vector of observations,
\( X \) - coefficient matrix of fixed effects,
\( b \) - vector of unknown fixed effects,
\( Z \) - coefficient matrix of random effects,
\( u \) - vector of unknown random effects,
\( e \) - random residual.

The specific form of the model is determined by the effects which enter the coefficient matrices \( X \) and \( Z \) and by the assumed nature of the variance structure. The expectations of random variables assumed below are almost universally used but the variance assumed is of a particular form. The variance of \( u \) is a scalar times the identity matrix, the variance of \( e \) is a general matrix \( R \), and no covariance is assumed between \( u \) and \( e \).

\[
\begin{bmatrix}
E \left[ \begin{array}{c} y \\ u \\ e \end{array} \right] & = & \begin{bmatrix} Xb \\ 0 \\ 0 \end{bmatrix} \\
\text{Var} \left[ \begin{array}{c} u \\ e \end{array} \right] & = & \begin{bmatrix} \sigma_u^2 & 0 \\ 0 & R \end{bmatrix}
\end{bmatrix}
\]

The identity variance structure for $u$ must be assumed to simplify the development of bounds. More complicated bound formulae arise when non-diagonal variances are allowed, such as when the animals to be evaluated are related. Using the variances and expectations specified, the mixed model equations for this model are in [1a].

\[
\begin{bmatrix}
X'R^{-1}X & X'R^{-1}Z \\
Z'R^{-1}X & Z'R^{-1}Z + (I_{\Omega_u}^2)^{-1}
\end{bmatrix}
\begin{bmatrix}
b \\
u
\end{bmatrix}
= \begin{bmatrix}
X'R^{-1}y \\
Z'R^{-1}y
\end{bmatrix}
\tag{1a}
\]

The variance of $e$ is often of the form $I_{\Omega_e}^2$ instead of $R$. The mixed model equations under this assumption are in [1b], with $k$ defined as the ratio $\sigma_e^2/\sigma_u^2$.

\[
\begin{bmatrix}
X'X & X'Z \\
Z'X & Z'Z + Ik
\end{bmatrix}
\begin{bmatrix}
b \\
u
\end{bmatrix}
= \begin{bmatrix}
X'y \\
Z'y
\end{bmatrix}
\tag{1b}
\]

Often it is advantageous to absorb the equations for fixed effects into the equations for random effects, such that the size of the remaining system depends only on the number of random elements. This development assumes that any equations for genetic groups are also absorbed, though this would not be the usual procedure. Defining $M$ as $I - X(X'X)^{-1}X'$, the reduced system is

\[
[Z'MZ + Ik] \hat{u} = Z'My.
\tag{2}
\]

Establishing bounds on diagonal elements of inverses

Prediction error variances (PEV) and accuracies of predictors ($r_{IH}^2$) are two related items normally desired by animal breeders whenever genetic evaluations are done. Some measure of accuracy of
information is essential for comparing alternative methods of analysis and for determining how much and what sorts of data to collect. Estimates of accuracy are also desired by the final users of genetic evaluations as an indicator of the potential change in the evaluation. Finally, VanRaden et al. (1984) have established that both the first and second moments of the evaluation are required in order to maximize genetic gain when selection is in multiple stages.

From results by Henderson (1975b), PEV and $r_{IH}^2$ may be shown to be functions of diagonal elements of the inverse of the coefficient matrix of [2]. If $t$ is a diagonal element of the inverse, PEV and $r_{IH}^2$ are equal to $t \sigma_e^2$ and $1-tk$, respectively (proof is given later). Simple bounds on $t$ may be established using partitioned matrices and positive definite or positive semi-definite quadratic forms. The basic strategy is to find formulae for diagonal elements of the inverse which involve quadratic forms of positive definite submatrices. Diagonal submatrices known to give either larger or smaller quadratic forms are then substituted for the actual submatrices to yield upper and lower bound formulae.

Throughout this manuscript comparisons will be made among variance matrices, and one matrix may be stated to be larger or smaller than another. The precise meaning is that any scalar quadratic form in $A$ (scalar refers to $A$ being pre- and post-multiplied by some vector, not some matrix) will be larger (or smaller) than any equivalent
quadratic form in $B$. This reduces to the definition that if $A$ minus $B$ is positive definite or semi-definite, then $A$ is said to be larger than $B$. If

$$x'Ax \geq x'Bx \quad \text{for all } x,$$

then

$$x'Ax - x'Bx \geq 0,$$

and

$$x'(A-B)x \geq 0.$$

Therefore, $A-B$ is positive semi-definite, and $A$ is "larger" than $B$, or $A \succ B$.

Three related properties worth remembering are: 1) for any positive definite matrix $P$, the matrix $P^{-1}$ is also positive definite, 2) if $A$ is larger than $B$ as defined above, then any submatrix along the diagonal of $A$ will be larger than the corresponding submatrix along the diagonal of $B$, and 3) if both $A$ and $B$ are positive definite and $A$ is larger than $B$, then $B^{-1}$ will be larger than $A^{-1}$. Proof of the first relationship is that if

$$x'Px > 0 \quad \text{for all } x \neq 0,$$

then

$$x'PP^{-1}Px > 0,$$

and

$$w'P^{-1}w > 0 \quad \text{for all } w \neq 0,$$

where $w = Px$.

Therefore, $P^{-1}$ is positive definite.

Proof of the second relationship is slightly more difficult. Suppose that $A_R$ is the submatrix of $A$ remaining when the first row and column of $A$ are excluded, and that $B_R$ is the equivalent submatrix of $B$. Also suppose that $A$ is larger than $B$ so that

$$x'Ax \geq x'Bx \quad \text{for all } x.$$
If this inequality holds for all vectors $x$ then it must hold for the subset of vectors $x$ which have 0 as their first element and $x_R$ as their remaining elements ($x'=[0 \ x_R]$).

\[
\begin{bmatrix}
0 & x_R
\end{bmatrix}
\begin{bmatrix}
a_{11} & a_{12} \\
a_{21} & A_R
\end{bmatrix}
\begin{bmatrix}
0 \\
x_R
\end{bmatrix}
\geq
\begin{bmatrix}
0 & x_R
\end{bmatrix}
\begin{bmatrix}
b_{11} & b_{12} \\
b_{21} & B_R
\end{bmatrix}
\begin{bmatrix}
0 \\
x_R
\end{bmatrix}
\]

This inequality holds for all $x_R$. Multiplying out this inequality simplifies to

\[
x_R A R x_R \geq x_R B R x_R \quad \text{for all } x_R.
\]

Thus, $A_R \geq B_R$.

Extensions of this logic can be used to prove that any submatrix along the diagonal of $A$ will be larger than the corresponding submatrix along the diagonal of $B$. Proof of the third relationship is more difficult and is given by Graybill (1983, p. 409).

The following partitioned matrix relationships are also essential for the development of bound formulae. Any square matrix $P$ may be partitioned into the segments shown in [3], where $P_{11}$ and $P_{22}$ are both also square. The inverse of $P$, if it exists, may be partitioned into these same segments and is represented in [4].

\[
P = \begin{bmatrix}
P_{11} & P_{12} \\
P_{21} & P_{22}
\end{bmatrix} \quad \text{[3]}
\]

\[
p^{-1} = \begin{bmatrix}
p_{11} & p_{12} \\
p_{21} & p_{22}
\end{bmatrix} \quad \text{[4]}
\]
For a positive definite $P$, the matrix $P^{-1}$ is guaranteed to exist as well as both $P_{11}^{-1}$ and $P_{22}^{-1}$. For matrices in which $P$, $P_{11}$, and $P_{22}$ are all invertible, the following two relationships are provided in many matrix algebra or statistics texts, for instance Hohn (1973, p. 78).

\[
P_{11}^{11} = [P_{11} - P_{12}P_{22}^{-1}P_{21}]^{-1}
\]
\[
P_{11}^{11} = P_{11}^{-1} + P_{11}^{-1}P_{12}P_{22}^{-2}P_{21}P_{11}^{-1}
\]

Relationships [5a] and [5b] become scalar relationships when $P$ is partitioned such that the first row and column are separated from the remainder of the matrix. This partitioning can be applied to the coefficient matrix in [2] to yield the partitioned matrix [6] and also the similarly partitioned form of its inverse [7].

\[
[Z'MZ + Ik] = \begin{bmatrix}
z_1'Mz_1 + k & z_1'MZ_R \\
z_R'Mz_1 & Z_R'MZ_R + Ik
\end{bmatrix}
\]

\[
[Z'MZ + Ik] = \begin{bmatrix}
D + k & d^- \\
d & Z_R'MZ_R + Ik
\end{bmatrix}
\]

where $Z = [z_1Z_R]$, 
\[D = z_1'Mz_1,\text{ and}\]
\[d^- = z_1'MZ_R.\]

\[
[Z'MZ + Ik]^{-1} = \begin{bmatrix}
t & q^- \\
q & Q^{-1}
\end{bmatrix}
\]
Because \( Z^\top M Z + I_k \) qualifies as a positive definite matrix, expressions [5a] and [5b] can be used to obtain exact equivalents for \( t \), which is the first diagonal element of the inverse. The first diagonal element was singled out merely for convenience of algebraic expression. Expressions for other diagonal elements can be obtained analogously but require partitioning the matrix into 9 segments instead of 4. This is because the row and column of interest would have to be separated from other rows and columns on both sides instead of just one side. Equations [8] and [9] follow from application of [5a] and [5b] to the coefficient matrix.

\[
\begin{align*}
t &= [D + k - d^\top (Z^\top R M Z_R + I_k)^{-1} d]^{-1} \\
t &= 1/(D + k) + d^\top Q^{-1} d/(D + k)^2
\end{align*}
\]

To obtain bounds on \( t \), it is necessary only to find quadratic forms known to be larger or smaller than those in the exact expressions. An obvious choice for a smaller quadratic form is to substitute the null matrix (\( \Phi \)) for \((Z^\top R M Z_R + I_k)^{-1}\) and \( Q^{-1} \) in expressions [8] and [9] respectively. This gives simply \( 1/(D + k) \) as the lower bound formula in both cases as shown in [10a] and [10b].

\[
\begin{align*}
t &\geq [D + k - d^\top (\Phi)d]^{-1} \\
t &\geq 1/(D + k) \\
t &\geq 1/(D + k) + d^\top (\Phi)d/(D + k)^2 \\
t &\geq 1/(D + k)
\end{align*}
\]
Another choice of a matrix smaller than both \((Z_R^T M_Z + I_k)^{-1}\) and \(Q^{-1}\) would be \((Z_R^T Z_T + I_k)^{-1}\). The matrix \(Z_R^T Z_T + I_k\) is diagonal with the number of progeny of a sire plus \(k\) as its diagonal elements. This makes it easy to obtain and to invert no matter what its size.

Proof that \((Z_R^T Z_T + I_k)^{-1}\) is smaller than the two matrices in the exact expressions is as follows, with the understanding that either \(Z\) or \(Z_R\) can be used in the following expressions with equal validity.

\[
\begin{align*}
Z^T M_Z + I_k &= Z^T [I - X(X^T X)^{-1} X] Z + I_k \\
Z^T M_Z + I_k &= Z^T Z + I_k - Z^T X(X^T X)^{-1} X^T Z \\
w^T (Z^T M_Z + I_k) w &= w^T (Z^T Z + I_k) w - w^T Z^T X(X^T X)^{-1} X^T Z w
\end{align*}
\]

The matrix \(X(X^T X)^{-1} X^T\) is symmetric idempotent for any choice of the generalized inverse \((X^T X)^{-1}\) (Kempthorne, 1983, p. 148) and all symmetric idempotent matrices are positive definite or positive semi-definite (Graybill, 1983, p. 419). Thus, the quadratic in \(X(X^T X)^{-1} X^T\) would be either positive or zero for any choice of \(w\) and therefore \(Z^T Z + I_k\) must be larger than \(Z^T M_Z + I_k\). The last step of the proof is the previously mentioned theorem that if \(A\) is larger than \(B\), then \(B^{-1}\) is larger than \(A^{-1}\).

\[
\begin{align*}
Z^T M_Z + I_k &\leq Z^T Z + I_k \\
(Z^T M_Z + I_k)^{-1} &\geq (Z^T Z + I_k)^{-1} \\
(Z_R^T M_Z + I_k)^{-1} &\geq (Z_R^T Z_T + I_k)^{-1}
\end{align*}
\]
Again, either $Z$ or $Z_R$ can be used in the above proof with equal validity. From the properties given earlier, if an entire matrix $(Z'Z + I_k)^{-1}$ is smaller than $(Z'MZ + I_k)^{-1}$, then any submatrix along the diagonal such as $(Z'Z_R + I_k)^{-1}$ must be smaller than the corresponding submatrix of $(Z'MZ + I_k)^{-1}$, which is $Q^{-1}$. Therefore $(Z'Z_R + I_k)^{-1}$ can be used as a smaller matrix than either $(Z'RZ_R + I_k)^{-1}$ or $Q^{-1}$ in expressions [8] and [9] to yield [10c] and [10d].

\[
\begin{align*}
t & \geq 1/[D + k - d'(Z'Z_R + I_k)^{-1}d] \quad [10c] \\
t & \geq 1/(D + k) + d'(Z'Z_R + I_k)^{-1}d/(D + k)^2 \quad [10d]
\end{align*}
\]

For ease of expression in some future developments, the notation $W = (Z'Z_R + I_k)^{-1}$ will be substituted. It may be helpful to think of $W$ as simply a diagonal matrix of weights. Expressions [10c] and [10d] can be rewritten with this substitution.

\[
\begin{align*}
t & \geq 1/(D + k - d'Wd) \quad [10c] \\
t & \geq 1/(D + k) + d'Wd/(D + k)^2 \quad [10d]
\end{align*}
\]

An intuitive argument as to why $(Z'Z + I_k)^{-1}$ should be smaller than $(Z'MZ + I_k)^{-1}$ is as follows. If the vector of fixed effects $b$ was known a priori instead of estimated from the data, $Xb$ could be subtracted from $y$ to yield equations for $\hat{u}$ given by

$$(Z'Z + I_k) \hat{u} = Z'(y - Xb).$$

Prediction error variance for $u$ obtained in this manner would be $(Z'Z + I_k)^{-1} \sigma^2_e$ instead of $(Z'MZ + I_k)^{-1} \sigma^2_e$ in the usual case when fixed effects are estimated from the data. It is appropriate to conclude
that PEV for \( \hat{u} \) should be smaller when fixed effects are known than when they are estimated and thus that the first matrix should be smaller than the second.

For upper bound formulae for \( t \), a matrix of the form \( Z'MZ + Ik \) (where \( Z'MZ \) is positive semi-definite) must be larger than simply \( Ik \). This is easy to demonstrate because

\[
\begin{align*}
    w'(Ik)w &= w'(Ik)w \quad \text{for all } w. \\
    \text{Also,} \quad w'(Ik)w &\leq w'(Ik)w + w'(Z'MZ)w, \\
    \text{and} \quad w'(Ik)w &\leq w'(Z'MZ + Ik)w. \\
    \text{Therefore,} \quad Ik \leq Z'MZ + Ik.
\end{align*}
\]

By previous argument, the inverse of \( Z'MZ + Ik \) must then be smaller than the inverse of \( Ik \) which is just \( Ik^{-1} \). Also, if this property holds for an entire matrix, then any square submatrix along the diagonal such as \( Q^{-1} \) will be smaller than the matrix \( Ik^{-1} \) with the same dimensions. Substituting \( Ik^{-1} \) into [8] and [9] leads to bounds [11a] and [11b].

\[
\begin{align*}
    t &\leq [D + k - d'(Ik^{-1})d]^{-1} \quad \text{[11a]} \\
    t &\leq 1/(D + k - d'd/k) \\
    t &\leq 1/(D + k) + d'(Ik^{-1})d/(D + k)^2 \\
    t &\leq 1/(D + k) + d'd/[k(D + k)^2] \quad \text{[11b]}
\end{align*}
\]

These expressions are easy to compute as they involve only the diagonal element \( (D + k) \) and the sum of squares of off-diagonal
elements \((d'd)\) weighted by the numbers of progeny of off-diagonal sires or divided by some function of \(D\) and \(k\). Formula \([\text{lla}]\) is an upper bound only if its denominator \((D + k - d'd/k)\) stays positive. As \(d'd/k\) approaches \(D+k\), \(t\) rises to plus infinity and then falls to negative infinity. Because of this bad behavior, \([\text{llb}]\) is suspected to be a better upper bound formula than \([\text{lla}]\). This hypothesis will be confirmed later.

The use of partitioned matrix relationships \([5a]\) and \([5b]\) led fairly straightforwardly to the lower bounds on \(t\) \([\text{10a to 10d}]\) and the upper bounds on \(t\) \([\text{lla}]\) and \([\text{llb}]\). Another set of bounds can be produced by a much more indirect route. Reasons for presenting this more complicated strategy are that it was the first method discovered by the author and that it leads to an upper bound uniformly better than the previous two. The third set of bounds is proven using a combination of relationships \([5a]\) and \([5b]\) and also a modification of the mixed model equations. A previous derivation by the author used selection index concepts but will not be presented here.

The close relationships between selection index theory, least squares, and BLUP such as described by Henderson (1963, 1978) provide a basis for development of the third set of bounds. Mixed model matrix \(F\) given in \([\text{12a}]\) is an altered form of \([\text{6}]\) in which \(k\) has not been added to the first diagonal element. Matrix \([\text{12a}]\) would result from the assumption that the first element of \(u\) is fixed and all others are random, but such assumption is not needed. The inverse of
[12a], if it exists, will be slightly different from the matrix [7] and is represented by [12b].

\[
F = \begin{bmatrix}
D & d^* \\
d & Z_MZ^* + Ik
\end{bmatrix}
\]  

[12a]

\[
F^{-1} = \begin{bmatrix}
t^* & q^* \\
q^* & Q^{-1}
\end{bmatrix}
\]  

[12b]

If matrix [12a] can be proven to be positive definite and hence invertible, the partitioned matrix results [5a] and [5b] may be applied. Matrix F is at least positive semi-definite as it can be formed as the sum of two positive semi-definite matrices. One of these is \(Z'MZ\) and the other is \(I*k\) which is just \(Ik\) with the first diagonal element set to zero, and \(k\) positive. F can be proven positive definite by demonstrating that there is no vector \(x\) other than \(x = 0\) such that \(x'Z'MZx\) and \(x'I*kx\) are simultaneously 0.

\[
F = Z'MZ + I*k
\]

\[
x'Fx = x'Z'MZx + x'I*kx
\]

\[
x'Fx = 0 \quad \Rightarrow \quad x'Z'MZx = 0,
\]

\[
x'I*kx = 0
\]

[13a]

Because both \(M\) and \(I*\) are symmetric idempotent, relationship [13a] can be rewritten as [13b] which in turn implies [13c]. Proof is similar to that found in Kempthorne (1983, p. 84).
\[ x'Fx = 0 \implies (x'Z'M)(MZx) = 0, \]
\[ k(x'I*)(I*x) = 0 \]  \[13b\]

\[ \implies MZx = 0, \ I*x = 0 \]
\[ \implies Z'MZx = 0, \ I*x = 0 \]  \[13c\]

For both conditions in [13c] to be true simultaneously, the null spaces of \( Z'MZ \) and \( I*k \) must overlap. A basis for the null space of \( I*k \) is a vector having 1 as the first element and 0's elsewhere. A basis for the null space of \( Z'MZ \) is a set of vectors \( s_i \) equal in number to the number of disconnected sire subsets, where each \( s_i \) has 1's corresponding to sires in that subset and 0's elsewhere. These two bases are linearly independent except when the first sire is his own disconnected subset. But this would mean he has no data ties to other sires and hence \( D \) would be zero. Because the two bases are independent, the null spaces are disjoint. Thus there are no values of \( x \) other than \( x = 0 \) that satisfy [13c] and \( F \) is proved to be positive definite for positive \( D \). Applying relationship [5a] to [12a] produces [14].

\[ t^* = 1/[D - d'(Z^R'MZ_R + Ik)^{-1}d] \]  \[14\]

The formula above for \( t^* \) is very similar to that for \( t \) in [8]. A direct relationship between \( t \) and \( t^* \) can be established using [8] and [14].
\[
\frac{t^*}{1 + t^*k} = \frac{1/[D - d^* (Z_RMZ_R + Ik)^{-1}d]}{1 + k/[D - d^* (Z_RMZ_R + Ik)^{-1}d]}
\]

Next multiply both the numerator and denominator by \([D - d^* (Z_RMZ_R + Ik)^{-1}d]\) to get

\[
t^*/(1 + t^*k) = 1/[D + k - d^*(Z_RMZ_R + Ik)^{-1}d],
\]

and \(t^*/(1 + t^*k) = t.\) \[15a\]

The derivative of \(t^*\) with respect to \(t^*\) is given by

\[
\frac{\partial t}{\partial t^*} = 1/(1 + t^*k)^2.\] \[15b\]

From [15a] and [15b], \(t^*\) is a uniformly increasing function of \(t^*\) for positive values of \(t^*\). Also, \(t^*\) is always positive because [12b] is positive definite. For these reasons, bounds which might be developed for \(t^*\) can be translated directly to bounds on \(t\) using [15a]. The bounds now considered for \(t^*\) are those produced when [5b] is applied to [12a] to yield

\[
t^* = 1/D + d^*Q^{-1}d/D^2.
\]

Limits for \(Q^{-1}\) will be the same as those for \(Q^{-1}\), namely \(\Phi \leq W \leq Q^{-1} \leq Ik^{-1}\). Using a partitioned matrix relationship analogous to [5a], \(Q^{-1}\) can be written as \([Z_RMZ_R + Ik - dd^*/D]^{-1}\). It follows that \((Z_RMZ_R + Ik)^{-1}\) or \(W\) should be smaller than \(Q^{-1}\) based on previous arguments. It follows also that \(Ik^{-1}\) should be larger than \(Q^{-1}\) if \(Z_RMZ_R - dd^*/D\) can be confirmed as a positive semi-definite matrix. But this term is just a submatrix of \(Z'MZ\) with the first row of \(Z'MZ\).
absorbed, so that it must be positive semi-definite just as Z'MZ is.
Substitution of these limits (Q, W, and Ik⁻¹) into the equality for t* produces bounds for t*.

\[ t^* \geq 1/D \]
\[ t^* \geq 1/D + d^\circ Wd/D^2 \]
\[ t^* \leq 1/D + d^\prime d/(D^2k) \]

Bounds for t using the relationship \( t = t^*/(1 + t^*k) \) are in [16a], [16b], and [17]. These follow directly from the three inequalities above. The lower bound [16a] is no different from those produced earlier in [10a] and [10b], but [16b] and [17] are different from those seen earlier.

\[ t \geq (1/D)/(1 + k/D) \]
\[ t \geq 1/(D + k) \]
\[ t \geq (1/D + d^\circ Wd/D^2)/(1 + k/D + k d^\circ Wd/D^2) \]
\[ t \geq (1 + d^\circ Wd/D)/(D + k + k d^\circ Wd/D) \]
\[ t \leq (1/D + d^\prime d/D^2k)/(1 + k/D + d^\prime d/D^2) \]
\[ t \leq (1 + d^\prime d/Dk)/(D + k + d^\prime d/D) \]

Comparison of bounds for t

Several different upper and lower bounds for t were developed ([10a to 10d], [11a], [11b], [16a], [16b], and [17], but only one upper and one lower bound would be sufficient to enclose the true value of t. The upper and lower bound formulae which yield numerical values closest to the true value for a particular sire would be the
formulae of choice for that sire. Using different formulae for different sires would not be convenient. The hypothesis tested here is that one upper or one lower bound formula might consistently outperform the others for any choice of k, for all possible data structures, and for all sires within a data structure. A pair of uniformly best bound formulae meeting these criteria would rule out any possible use for the others if all were equally easy to compute.

The three upper bounds for t ([11a], [11b], and [17]) will be compared first. These are all functions of the same three terms from the mixed model equations, namely D, k, and \( d'd \). Proving that one function lies above or below another over all valid choices of D, k, and \( d'd \) is a four-dimensional problem. Valid choices for D, k, and \( d'd \) are described by the following inequalities: \( D > 0, k > 0, 0 < d'd < D^2 \). The four-dimensional problem can be reduced to two dimensions by taking D and k to be arbitrary positive constants.

By substituting 0 for \( d'd \) in [11a], [11b], and [17], the three bounds can all be shown to converge to \( 1/(D + k) \) as \( d'd \) approaches 0. This happens to be a boundary point for \( d'd \). Given that the functions coincide at a boundary point, a function with consistently higher first derivative will always lie above the others barring any discontinuities in the functions compared. Partial derivatives of the three bound functions with respect to \( d'd \) are in [18-20].
\[ \frac{\partial[11a]}{\partial d'd} = \frac{1/k}{(D + k - d'd/k)^2} \]  \[ \text{[18]} \]

\[ \frac{\partial[11b]}{\partial d'd} = \frac{1/k}{(D + k)^2} \]  \[ \text{[19]} \]

\[ \frac{\partial[17]}{\partial d'd} = \frac{1/k}{(D + k + d'd/D)^2} \]  \[ \text{[20]} \]

Derivative [19] is a constant with respect to \(d'd\), which means that [11b] is a linear function of \(d'd\). Derivative [20] is smaller than [19] for all positive values of \(d'd\). Derivative [18] is larger than [19] for most reasonable values of \(d'd\), but becomes infinite at the point of discontinuity of [11a]. This point is where \(d'd/k = D + k\). The behavior of these curves is demonstrated in Figure 1, which shows clearly that expression [17] provides the best upper bound for \(t\). Because these relationships are true for arbitrary positive choices of \(D\) and \(k\), they are true for all choices and combinations of positive values of \(D\) and \(k\).
$D=20$, $k=10$, $d\cdot d$ ranges from 0 to $D^2$.

2 $[11a]$ diverges to positive and negative infinity at $d\cdot d=300$.

3 True values of $t$ lie between $[10a]$ and $[17]$, as $[10a]$ is a lower bound.

The lower bounds on $t$ ([$10a$ to $10d$], $[16a]$, and $[16b]$) can be compared in a similar manner. Three of these bounds ([$10a$], $[10b]$, and $[16a]$) are identical and will be referred to as simply $[10a]$.

The remaining three bounds involve $d\cdot W_d$ and are just slightly more difficult to compute than either $[10a]$ or the upper bound formulae. Derivatives of the lower bound expressions with respect to $d\cdot W_d$ are in [21 to 24].
Like the upper bound formulae, the four lower bounds will coincide at \( 1/(D + k) \) when \( d \cdot Wd \) is zero. Derivatives [21 to 24] can be ranked by inspection from lowest to highest as [21], [24], [23], and [22]. As evidenced by its higher first derivative, [10c] then lies above the other lower bounds for all valid choices of \( D, k, \) and \( d \cdot Wd \). Valid choices for \( d \cdot Wd \) can be shown to lie in the interval \( 0 \leq d \cdot Wd \leq D^2/(D + k) \), while \( D \) and \( k \) are again any positive real values. This makes [10c] a better bound choice, because the true values of \( t \) will lie closer to this bound than to the others. Expression [10c] is not, however, as easy computationally as [10a] and thus [10a] might sometimes be preferred for its simplicity. The respective upper and lower bounds [17] and [10c] have then proved to be universally superior to the others in terms of tightness, while [10a] remains of interest.
as a bound not as tight but simpler. The lower bounds are diagrammed in Figure 2.

Figure 2. Behavior of lower bounds for $t^1$

$^1D=20, k=10, d^{-Wd}$ ranges from 0 to $D^2/(D + k)$.

Bounds for accuracy and prediction error variance

So far only bounds on $t$ and not on PEV or accuracy have been developed. Bounds on PEV follow directly from those on $t$ as PEV is simply $t\sigma_e^2$ (Henderson, 1975b). Bounds on $r_{IH}^2$ are only slightly more difficult to produce but will be listed for ease of reference. Accuracy is the proportion of genetic variance explained by the predictor and is the following function of $t$. 
\[ r_{IH}^2 = \frac{\sigma_u^2}{\sigma_u^2} \]
\[ r_{IH}^2 = \frac{(\sigma_u^2 - t \sigma_e^2)}{\sigma_u^2} \]
\[ r_{IH}^2 = 1 - tk \]

A uniformly superior bound on \( t \) must translate to a uniformly superior bound on \( r_{IH}^2 \) as well. For this reason, only the three most useful bounds mentioned previously will be translated to bounds on \( r_{IH}^2 \). Relationships \([25a\text{ to }25c]\) follow from bounds on \( t \) given in \([10a]\), \([10c]\), and \([17]\). Directions of the inequalities of the bounds have changed because \( r_{IH}^2 \) is a negative function of \( t \).

\[
\begin{align*}
    r_{IH}^2 &\leq 1 - k[1/(D + k)] \\
    r_{IH}^2 &\leq D/(D + k) \quad \text{[25a]} \\
    r_{IH}^2 &\leq 1 - k[1/(D + k - d\cdot Wd)] \\
    r_{IH}^2 &\leq (D - d\cdot Wd)/(D + k - d\cdot Wd) \quad \text{[25b]} \\
    r_{IH}^2 &\geq 1 - k[(1 + d\cdot d/Dk)/(D + k + d\cdot d/D)] \\
    r_{IH}^2 &\geq D/(D + k + d\cdot d/D) \quad \text{[25c]}
\end{align*}
\]

**Example of bound computations**

A small numerical example of bound computations will be used to demonstrate the technique and also to point out an interesting property
of one of the bounds. The example data set will have three progeny of each of three sires in just one herd. Absorbing the herd equation produces the coefficient matrix below.

\[
Z^\prime MZ = \begin{bmatrix}
2 & -1 & -1 \\
-1 & 2 & -1 \\
-1 & -1 & 2
\end{bmatrix}
\]

Using a value of 3 for \(k\), the matrix \(Z^\prime Z + Ik\) would be comprised of 6's on the diagonal and 0's elsewhere. Likewise, \((Z^R_R + Ik)^{-1}\) or \(W\) would have elements equal to 1/6 on the diagonal and 0's elsewhere. For each of the three sires, then, \(D = 2\), \(d^\prime d = (-1)^2 + (-1)^2 = 2\), and \(d^\prime Wd = (-1)^2/6 + (-1)^2/6 = .3333\). Adding the ratio \(k = 3\) to the diagonals of \(Z^\prime MZ\) would result in the following matrix.

\[
Z^\prime MZ + Ik = \begin{bmatrix}
5 & -1 & -1 \\
-1 & 5 & -1 \\
-1 & -1 & 5
\end{bmatrix}
\]

Bounds for \(t\) are produced with the relationships \(t \geq 1/(D + k)\), \(t \geq 1/(D + k - d^\prime Wd)\), and \(t \leq (1 + d^\prime d/[Dk])/(D + k + d^\prime d/D)\) which were seen in [10a], [10c], and [17]. For each of the three sires, numerical bounds are given by:

\[
\begin{align*}
t &\geq 1/(2 + 3) = 1/5 = .2 \\
t &\geq 1/(2 + 3 - .3333) = .2143 \\
t &\leq (1 + 2/[2*3])/(2 + 3 + 2/2) = .2222
\end{align*}
\]
Actual values of $t$ are the diagonal elements of the inverse of $Z' M Z + I_k$.

$$(Z' M Z + I_k)^{-1} = \begin{bmatrix} .2222 & .0556 & .0556 \\ .0556 & .2222 & .0556 \\ .0556 & .0556 & .2222 \end{bmatrix}$$

It is interesting that these actual values for $t$ are identical to those produced by the upper bound formula for $t$. Whenever data are balanced, as in this example, [17] produces exact values of $t$. This can be proven algebraically using formulae presented by Graybill (1983, p. 190) for matrices of this type. Expression [17] also produces exact values when the data consists of balanced subsets of sires. An example of balanced subsets would be to add to the above data set a new herd having equal numbers of progeny on a new group of sires. This new group of sires would be a new balanced subset, and no data ties can occur between subsets for [17] to produce exact answers.

In unbalanced data, the true value of $t$ drifts away from the upper bound formula in the direction of the lower bounds. In terms of the graph in Figure 1, all values of $t$ would lie directly on curve [17] for data which was balanced or in balanced subsets. For data ranging from almost balanced to very unbalanced, true values of $t$ would drift away from curve [17] toward the direction of the lower bound [10a].

Bounds for accuracy computed with formulae [25a to 25c] for the first data set discussed are given below. True accuracy for the three sires was .3333.
\[ r_{IH}^2 \leq 2/(2 + 3) = 2/5 = .4 \]

\[ r_{IH}^2 \leq (2 - .333)/(2 + 3 - .333) = .3571 \]

\[ r_{IH}^2 \geq 2/(2 + 3 + 2/2) = 1/3 = .3333 \]

An intuitive argument as to why bounds can be developed is as follows. In Gauss-Seidel iteration, the solution for the first sire is expressed as a function of the first right-hand side \((z_iMy)\), the coefficients for other sires \((d')\), and the solutions for other sires \((\hat{u}_R)\) by the equation

\[ \hat{u}_1 = (z_iMy - d\hat{u}_R)/(D + k). \]

From this, it is evident that the variance of \(\hat{u}_1\) could be expressed as a function of \(d'\text{Var}(\hat{u}_R)\). Bounds are obtained when one realizes that there are limits to the variance of \(\hat{u}_R\). An upper limit occurs when complete information exists for these off-diagonal sires, such that \(\text{Var}(\hat{u}_R) = I\sigma_u^2\). A lower limit occurs when no information exists for these other sires, in which case a null matrix is substituted for \(\text{Var}(\hat{u}_R)\).
RESULTS AND DISCUSSION

Deriving bounds and proving that they indeed enclose some sought-after true value is one step removed from showing that these bounds are useful in ordinary situations. For example, it is already known that accuracies are bounded by the values 0 and 1, but this is of no aid in describing how much information a particular sire possesses. The usefulness of a set of bounds relates directly to how tightly the true values are enclosed.

To investigate tightness of the bounds, an example data set was created which mimicked the data pattern usually seen in dairy sire evaluation. The model included only herds and sires, with herds treated as fixed and absorbed. Sires and errors were uncorrelated, with variance structures $I\sigma^2_s$ and $I\sigma^2_e$, respectively. Three different ratios of error to sire variance ($k$) were used in the example to allow inference to various traits of interest. Ratios used for $\sigma^2_e/\sigma^2_s$ were 7, 15, and 79, corresponding to heritabilities of .50, .25, and .05. This range should include nearly all traits of interest to animal breeders.

To appear realistically large and yet to avoid excessive computation costs, the generated data set included 100 sires with a total of 12,630 daughters distributed across 400 herds. Data from the same 100 sires were used for the three $k$ values. The number of daughters of any particular sire in any particular herd was generated as an approximate Poisson random variable. This insured that sires were used
randomly with respect to each other and with respect to herds. Sires were intentionally given different numbers of daughters to provide for a wide range of accuracies. Maximum was 507 daughters in 151 herds; minimum was 6 daughters in 6 herds.

Results of the simulation were very encouraging. Accuracies for most sires were enclosed by bounds plus or minus about one percent of the true value of accuracy when a value of 15 was used for $k$. Maximum and minimum distances between bounds for accuracy of a sire were .0178 and .0023, respectively, for $k = 15$. With $k = 7$, accuracies were larger and bounds wider, while $k = 79$ produced smaller accuracies with tighter bounds. These tighter bounds with larger values of $k$ are explained by the increased size of diagonal relative to off-diagonal elements.

Examples of bounds along with true values of accuracy for a sample of sires using the three different $k$ are in Table 1. Upper and lower bounds were those given in [25a] and [25c], while true values were obtained by inversion of the coefficient matrix. Accuracies were enclosed within a usefully small range for all sires in the data set and for values of $k$ ranging from 7 to 79. Differences between the bounds as a percentage of true accuracy were nearly the same for all sires compared. These results are encouraging, but should not be overly surprising because one of the bounds (the reciprocal of the diagonal element) is already widely used and is known to be a good approximation, though it was not previously known to be a bound.
Table 1. Performance of bounds in simulated sire evaluation for a sample of sires

<table>
<thead>
<tr>
<th>Sire No.</th>
<th>Dtrs.</th>
<th>Herds</th>
<th>( r^2_{\text{IH}} )</th>
<th>( \text{Bounds} )</th>
<th>( \text{Difference} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Lower</td>
<td>Upper</td>
</tr>
<tr>
<td>1</td>
<td>336</td>
<td>118</td>
<td>.9666</td>
<td>.9597</td>
<td>.9771</td>
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<tr>
<td>25</td>
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<td>69</td>
<td>43</td>
<td>35</td>
<td>.8461</td>
<td>.8399</td>
<td>.8541</td>
</tr>
<tr>
<td>93</td>
<td>12</td>
<td>6</td>
<td>.6100</td>
<td>.6021</td>
<td>.6168</td>
</tr>
<tr>
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<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( k = 7 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>336</td>
<td>118</td>
<td>.9416</td>
<td>.9356</td>
<td>.9522</td>
</tr>
<tr>
<td>25</td>
<td>191</td>
<td>94</td>
<td>.9113</td>
<td>.9059</td>
<td>.9212</td>
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<td>35</td>
<td>.7258</td>
<td>.7216</td>
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<tr>
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<td></td>
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<td>.7793</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>( k = 79 )</td>
<td></td>
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</tbody>
</table>

The data set generated seems sufficiently similar to actual sire evaluation data to indicate that the method of bounds would perform well in a real data set of this size. The bounds, however, were not developed to be used in evaluations of only 100 sires, where direct inversion is possible. It is in the largest evaluations that the bounds would give greatest computational advantage. But will the bounds stay as tight as sire numbers increase? Fortunately, they may be even tighter in larger systems. The larger the number of other sires that a particular sire has data ties to, the smaller is \( d/d \) compared to \( D \), and the bounds converge.
One reservation about drawing inferences from these results to real data situations is that the simulation considered only a simple mixed model with one random effect, no interaction, identity variance structures for u and e, and all fixed effects absorbed. These restrictions were required because the proofs and methodology necessary to obtain bounds for more complex models were not developed in this manuscript. Because of the increasing interest in more sophisticated models and the very large data sets to be evaluated, procedures for extending this concept of bounds to a broader range of models would probably have a high payoff.

An even larger payoff might result from extending the method of bounds to estimation of variance components. Algorithms for computing MIVQUE or REML estimates of variance components require computing traces of large inverses. Obviously, if bounds can be obtained for individual diagonal elements of an inverse, then a sum of upper or lower bounds on individual diagonal elements would constitute an upper or lower bound on the sum, which is the trace. In this manner, upper and lower bounds might be computed on MIVQUE and REML estimates of variance components for far less than the cost of obtaining exact estimates through matrix inversion. This topic, however, is much too broad to be adequately treated in this manuscript. Preliminary results indicate that the approach using bounds does well in a simple model and in fact was superior to Henderson's Simple Method in the data set considered.
SUMMARY AND CONCLUSIONS

Diagonal elements of inverses of large coefficient matrices are often required by animal breeders to report accuracies, to report prediction error variances, and to estimate variance components by methods such as MIVQUE or REML. Computing such inverses is often either impossible or prohibitively expensive for very large data sets. For models without relationships, bounds on diagonal elements of an inverse may be computed using simple functions of elements of the original coefficient matrix. Bounds are proven using partitioned matrix relationships and positive definite quadratic forms.

A total of seven different bounds were developed using three different strategies which involved two well-known partitioned matrix relationships. Three lower bounds were developed utilizing the sum of squares of off-diagonal elements weighted by numbers of progeny of the off-diagonal sire plus k. Another lower bound was simply the reciprocal of the original diagonal element. Three different upper bounds were also established, all involving the original diagonal element and the sum of squares of off-diagonal elements.

Of the three upper bound formulae, one was proven to be superior to the other two for all sires, for all data sets, and for all choices of k. One of the four lower bounds was also declared to be universally superior to the others, though not all of the lower bounds were equally easy to compute. All of these bounds, however, are computationally far simpler than inversion.
The two formulae used for computing upper and lower bounds on $r_{IH}^2$ were $D/(D + k)$ and $D/(D + k + d^2/dD)$, respectively, where $D$ is a diagonal element of $Z'MZ$, $d^2$ is the sum of squares of off-diagonal elements in that row, and $k$ is the ratio $\sigma^2_e/\sigma^2_s$. These two bounds enclosed the accuracies of most sires in about a one-percentage-point range for a simulated data set with $k = 15$. These bounds have the interesting property of becoming tighter as the data set grows larger when sires are used randomly with respect to each other. The bounds were already tight enough to be considered very useful in a data set having only 100 sires and 400 herds.

The bounds presented in this manuscript may prove to be a very effective and efficient approximation procedure for animal breeders working with large sets of mixed model equations. A severe limitation of the results presented are that they pertain only to the fairly simplistic model assumed. Extensions of the procedure of bounds might be made to models with more than one random effect, models with non-diagonal variance structures for $u$ such as when relationships are included, multi-trait models with covariance components, and models with some fixed effects not absorbed, such as with genetic groups. It is hoped that extensions of the procedure of bounds to other models will lead to formulae as easy to compute and as useful as those seen here.
REFERENCES CITED


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