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Variance component estimation techniques compared for two mating designs with forest genetic architecture through computer simulation

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Abstract Computer simulation was used to compare minimum variance quadratic estimation (MIVQUE), minimum norm quadratic unbiased estimation (MINQUE), restricted maximum likelihood (REML), maximum likelihood (ML), and Henderson's Method 3 (HM3) on the basis of variance among estimates, mean square error (MSE), bias and probability of nearness for estimation of both individual variance components and three ratios of variance components. The investigation also compared three procedures for dealing with negative estimates and included the use of both individual observations and plot means as the experimental unit of the analysis. The structure of data simulated (field design, mating designs, genetic architecture and imbalance) represented typical analysis problems in quantitative forest genetics. Results of comparing the estimation techniques demonstrated that: estimates of probability of nearness did not discriminate among techniques; bias was discriminatory among procedures for dealing with negative estimates but not among estimation techniques (except ML); sampling variance among estimates was discriminatory among procedures for dealing with negative estimates, estimation techniques and unit of observation; and MSE provided no additional information to variance of the estimates. HM3 and REML were the closest competitors under these criteria; however, REML demonstrated greater robustness to imbalance. Of the three negative estimate procedures, two are of practical significance and guidelines for their application are presented. Estimates from individual observations were always preferable to those from plot means over the experimental levels of this study.

Key words Minimum · Norm · Restricted · Likelihood · Half-diallel

Introduction

In many applications of quantitative genetics, geneticists are commonly faced with the analysis of field data containing a multitude of flaws (e.g., non-normality, imbalance, and heteroscedasticity). Imbalance, as one of these flaws, is intrinsic to quantitative forest genetics research because of the difficulty in making crosses for full-sib tests and the biological realities of long-term field experiments. Few definitive studies have been conducted to establish optimal methods for the estimation of variance components from unbalanced data. Simulation studies using simple models (one-way or two-way random models) have been conducted for certain data structures, namely imbalance, experimental design, and variance parameters (Corbeil and Searle 1976; Swallow and Monahan 1984; interpretations by Littell and McCutchan 1986). The results from these studies indicate that technique optimality is a function of the data structure.

In practice (both historically and still commonplace), estimation of variance components in forest genetics applications has been achieved by sequentially adjusted sums of squares as an application of Henderson's Method 3 (HM3, Henderson 1953). Under normality, and with balanced data, this technique has the desirable properties of being the minimum variance unbiased estimator. If the data are unbalanced, then the only property retained by HM3 estimation is unbiasedness (Searle 1971, 1987 pp 492, 493, 498). Other estimators have been shown to be locally superior to HM3 in

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variance or mean square error properties in certain cases (Klotz et al. 1969; Olsen et al 1976; Swallow 1981; Swallow and Monahan 1984).

Over the last 25 years, there has been a proliferation of variance component estimation techniques including minimum norm quadratic unbiased estimation (MINQUE, Rao 1971a), minimum variance quadratic unbiased estimation (MIVQUE, Rao 1971b), maximum likelihood (ML, Hartley and Rao 1967), and restricted maximum likelihood (REML, Patterson and Thompson 1971). The practical application of these techniques has been impeded by their computational complexity. However, with continuing advances in computer technology and the appearance of better computational algorithms, the application of these procedures continues to become more tractable (Harville 1977; Giesbrecht 1983; Meyer 1989). Whether these methods of analysis are superior to HM3 for many genetics applications remains to be demonstrated.

With balanced data and disregarding negative estimates, all previously mentioned techniques except ML produce the same estimates (Harville 1977). With unbalanced data, each technique produces a different set of variance component estimates. Criteria must then be adopted to discriminate among techniques. Candidate criteria for discrimination include unbiasedness (large number convergence on the parametric value), minimum variance (estimator with the smallest sampling variance), minimum mean square error (minimum of sampling variance plus squared bias, Hogg and Craig 1978), and probability of nearness (probability that sample estimates occur in a certain interval around the parametric value, Pitman 1937).

Negative estimates are also problematic in the estimation of variance components. Five alternatives for dealing with the dilemma of estimates less than zero (outside the natural parameter space of zero to infinity) are (Searle 1971): (1) accept and use the negative estimate, (2) set the negative estimate to zero (producing biased estimates), (3) re-solve the system with the offending component set to zero, (4) use an algorithm which does not allow negative estimates, and (5) use the negative estimate to infer that the wrong model was utilized.

The purpose of this research was to determine if the criteria of unbiasedness, minimum variance, minimum mean square error, and probability of nearness, discriminated among variance component estimation techniques while exploring various alternatives for dealing with negative variance component estimates. In order to make such comparisons, a large number of data sets were required for each experimental level. Using simulated data, this paper compares variance component estimation techniques for plot-mean and individual observations, two mating systems (modified half-diallel and half-sib), and two sets of parametric variance components. Types of imbalance and levels of factors were chosen to reflect common situations in forest genetics.

Methods

Experimental approach

The overall experimental design for the simulation was originally conceived as a factorial with two types of mating design, two sets of true variance components spanning the range of commonly reported values for growth traits in conifers (Table 1), and two kinds of observations (individual and plot mean). There were three types of imbalance: (1) different survival levels (80% and 60%, with 80%, representing moderate survival and 60% representing poor survival); (2) for full-sib designs three levels of missing crosses (0, 2, and 5 out of 15 crosses); and (3) for half-sib designs two levels of connectedness among tests (15 and 10 common families between tests out of 15 families per test). Because of computational time constraints, the experiment could not be run as a complete factorial and the investigation continued as a partial factorial. In general, the approach was to run levels which were at opposite ends of the imbalance spectrum, i.e., 80% survival and no missing crosses versus 60% survival and five missing crosses, within a variance component level. If results were consistent across these treatment combinations, intermediate levels were not run.

Designation of a treatment combination is by a five-character alpha-numeric field. The first character is either "H" (half-sib) or "D" (half-diallel). The second character denotes the set of parametric variance components where "1" designated the set of variance components associated with heritability equalling 0.1 and "2" designated the set of variance components associated with heritability equalling 0.25 (Table 1). The third character is an "S" indicating that the last two characters determine the imbalance level. The fourth character designates the survival level either "6" for 60% or "8" for 80%. The final character specifies the number of missing crosses (half-diallel) or lack of connectedness (half-sib).

Table 1 Sets of true variance components for the half-diallel and half-sib mating designs generated from specification of two levels of single-tree heritability (h^2), type B correlation (r_B), and non-additive to additive variance ratio (d/a)

Genetic ratios[b]			Mating design	True variance components[b]							
h^2	r_B	d/a		σ_t^2	σ_b^2	σ_g^2	σ_s^2	σ_{tg}^2	σ_{ts}^2	σ_p^2	σ_w^2
0.1	0.5	1.0	Full-sib	1.0	0.5	0.25	0.25	0.25	0.25	0.595	7.905
0.25	0.8	0.25	Half-sib	1.0	0.5	0.25	NA	0.25	NA	0.475	7.9964
			Full-sib	1.0	0.5	0.625	0.1562	0.1562	0.0391	0.5769	7.6649

[a] $h^2 = 4\sigma_g^2/\sigma_{\text{phenotypic}}^2$; $r_B = 4\sigma_g^2/(4\sigma_g^2 + 4\sigma_{tg}^2)$; and σ_D^2/σ_A^2 as $d/a = 4\sigma_s^2/4\sigma_g^2$

[b] See definitions in equation 1

Experimental design for simulated data

The mating design for the simulation was either a six-parent half-diallel (no selfs) or a 15-parent half-sib. The randomized complete block field design was in three locations with four complete blocks per location and six trees per family in a block; where family is a full-sib family for half-diallel, or a half-sib family for the half-sib design. This field design and the mating designs reflect typical designs in forestry applications (Squillace 1973; Wilcox et al. 1975; Bridgwater et al. 1983; Weir and Goddard 1986; Loo-Dinkins et al. 1990) and are also commonly used in other disciplines (Matzinger et al. 1959; Hallauer and Miranda 1981; Singh and Singh 1984). The six trees per family could be considered as contiguous or non-contiguous plots without affecting the results or inferences.

Full-sib linear model. The scalar linear model employed for half-diallel individual observations is

$$y_{ijklm} = \mu + t_i + b_{ij} + g_k + g_l + s_{kl} + tg_{ik} + tg_{il} + ts_{ikl} + p_{ijkl} + w_{ijklm} \quad (1)$$

where y_{ijklm} is the m-th observation of the kl-th cross in the j-th test;
- μ is the population mean;
- t_i is the random variable test environment $\sim$ NID $(0, \sigma_t^2)$;
- b_{ij} is the random variable block $\sim$ NID $(0, \sigma_b^2)$;
- g_k is the random variable female general combining ability (gca) $\sim$ NID $(0, \sigma_g^2)$;
- g_l is the random variable male gca $\sim$ NID $(0, \sigma_g^2)$;
- s_{kl} is the random variable specific combining ability (sca) $\sim$ NID $(0, \sigma_s^2)$;
- tg_{ik} is the random variable test by female gca interaction $\sim$ NID $(0, \sigma_{tg}^2)$;
- tg_{il} is the random variable test by male gca interaction $\sim$ NID $(0, \sigma_{tg}^2)$;
- ts_{ikl} is the random variable test by sca interaction $\sim$ NID $(0, \sigma_{ts}^2)$;
- p_{ijkl} is the random variable plot $\sim$ NID $(0, \sigma_p^2)$;
- w_{ijklm} is the random variable within-plot $\sim$ NID $(0, \sigma_w^2)$; and there is no covariance between random variables in the model.

This linear model in matrix notation is (dimensions below model component)

$$\underset{nx1}{\mathbf{y}} = \underset{nx1}{\mu\mathbf{1}} + \underset{nxt\ tx1}{\mathbf{Z_T e_T}} + \underset{nxb\ bx1}{\mathbf{Z_B e_B}} + \underset{nxg\ gx1}{\mathbf{Z_G e_G}} + \underset{nxs\ sx1}{\mathbf{Z_S e_S}} + \underset{nxtg\ tgx1}{\mathbf{Z_{TG} e_{TG}}} + \underset{nxts\ tsx1}{\mathbf{Z_{TS}\, e_{TS}}} + \underset{nxp\ px1}{\mathbf{Z_P e_P}} + \underset{nx1}{\mathbf{e_W}} \quad (2)$$

where $\mathbf{y}$ is the observation vector;
- $\mathbf{Z_i}$ is the portion of the design matrix for the ith random vector;
- $\mathbf{e_i}$ is the vector of unobservable random effects for the ith random variable;
- $\mathbf{1}$ is a vector of 1's; and
- n, t, b, g, s, tg, ts, and p are the number of observations, tests, blocks, gcas, gcas, scas, test by gca interactions, test by sca interactions and plots, respectively.

Utilizing customary assumptions in half-diallel mating designs (Method 4, Griffing 1956), the variance of an individual observation is

$$\mathrm{Var}(y_{ijklm}) = \sigma_t^2 + \sigma_b^2 + 2\sigma_g^2 + \sigma_s^2 + 2\sigma_{tg}^2 + \sigma_{ts}^2 + \sigma_p^2 + \sigma_w^2; \quad (3)$$

and in matrix notation the variance-covariance matrix for the observations is

$$\mathrm{Var}(y) = \mathbf{Z_T Z_T'}\sigma_t^2 + \mathbf{Z_B Z_B'}\sigma_b^2 + \mathbf{Z_G Z_G'}\sigma_g^2 + \mathbf{Z_S Z_S'}\sigma_s^2 + \mathbf{Z_{TG} Z_{TG}'}\sigma_{tg}^2 + \mathbf{Z_{TS} Z_{TS}'}\sigma_{ts}^2 + \mathbf{Z_P Z_P'}\sigma_p^2 + \mathbf{I_n}\sigma_w^2 \quad (4)$$

where "′" indicates the transpose operator, all matrices of the form $\mathbf{Z_i Z_i'}$ are nxn, and $\mathbf{I_n}$ is an nxn identity matrix.

Half-sib linear model. The scalar linear model for half-sib individual observations is

$$y_{ijkm} = \mu + t_i + b_{ij} + g_k + tg_{ik} + p_{ijk}^h + w_{ijkm}^h \quad (5)$$

where y_{ijkm} is the m-th observation of the k-th half-sib family in the jth block of the i-th test;
- μ, t_i, b_{ij}, g_k, and tg_{ik} retain the definition in equation 1;
- p_{ijk}^h is the random variable plot containing different genotype-by-environment components than equation 1 $\sim$ NID$(0, \sigma_{ph}^2)$;
- w_{ijkm}^h is the random variable within-plot containing different levels of genotypic and genotype-by-environment components than equation 1 $\sim$ NID$(0, \sigma_{wh}^2)$; and there is no covariance between random variables in the model.

The variance of an individual observation in half-sib designs is

$$\mathrm{Var}(y_{ijkm}) = \sigma_t^2 + \sigma_b^2 + \sigma_g^2 + \sigma_{tg}^2 + \sigma_{ph}^2 + \sigma_{wh}^2, \quad (6)$$

and

$$\mathrm{Var}(\mathbf{y}) = \mathbf{Z_T Z_T'}\sigma_t' + \mathbf{Z_B' Z_B}\sigma_b^2 + \mathbf{Z_G Z_G'}\sigma_g^2 + \mathbf{Z_{TG} Z_{TG}'}\sigma_{tg}^2 + \mathbf{Z_P Z_P'}\sigma_{ph}^2 + \mathbf{I_n}\sigma_{wh}^2. \quad (7)$$

For an observational vector based on plot means, the plot and within-plot random variables were combined by taking the arithmetic mean across the observations within a plot. The resulting plot-means model has a new σ_p^2 or $\sigma_{ph}^2(\sigma_{p*}^2$ or $\sigma_{ph*}^2)$ term being a composite of the plot and within-plot variance terms of the individual observation model.

Three estimates of ratios among variance components were determined: (1) single tree heritability adjusted for test environment and block as $\hat{h}^2 = 4\hat{\sigma}_g^2/\hat{\sigma}_{\text{phenotypic}}^2$, where $\hat{\sigma}_{\text{phenotypic}}^2$ is the estimate of the variance of an individual observation with the variance components for test environment and block removed; (2) type B correlation as $\hat{r}_B = 4\hat{s}_g^2/(4\hat{\sigma}_g^2 + 4\hat{\sigma}_{tg}^2)$; and (3) dominance to additive variance ratio as $d/a = 4\hat{\sigma}_s^2/4\hat{\sigma}_g^2$.

Data generation and deletion

Data generation was accomplished by using a Cholesky decomposition of the variance-covariance matrix for the observations (Goodnight 1979) and a vector of pseudo-random standard normal deviates generated using the Box-Muller transformation and pseudo-random uniform deviates (Knuth 1981; Press et al. 1989). The upper-lower decomposition creates a matrix ($\mathbf{U}$) with the property that $\mathrm{Var}(\mathbf{y}) = \mathbf{U'U}$. The vector of pseudo-random standard normal deviates ($\mathbf{z}$) has a variance-covariance matrix equal to an indentity matrix ($\mathbf{I_n}$) where $\mathbf{n}$ is the number of observations. The vector of observations is created as $\mathbf{y} = \mathbf{U'}z$. Then $\mathrm{Var}(\mathbf{y}) = \mathbf{U'}(\mathrm{Var}(\mathbf{z}))\mathbf{U}$ and since $\mathrm{Var}(\mathbf{z}) = \mathbf{I_n}$, $\mathrm{Var}(\mathbf{y}) = \mathbf{U'IU} = \mathbf{U'U}$.

Analyses of survival patterns [data from the Cooperative Forest Genetic Research Program (CFGRP) at the University of Florida] were used to develop survival distributions for use in the simulation. The data sets chosen for survival analysis were from full-sib slash pine (*Pinus elliottii* var. *elliottii* Engelm) tests. Survival levels for most crosses clustered around the average value; however, there were always a few crosses that had much poorer survival than average and also a small number of crosses that had much better survival than average. Thus, a lower than average survival level was arbitrarily assigned to certain crosses, a higher than average survival level was assigned to certain crosses, and the average survival level assigned to most crosses. This modelling of survival pattern was also extended to the half-sib mating design. At 80% survival no missing plots were allowed and at 60% survival missing plots occurred at random.

Full-sib family deletion simulated crosses which could not be made and were, therefore, missing from the experiment. The deletion was restricted in the five missing cross simulations to a maximum of four crosses per parent to prevent loss of all the crosses in which a single parent appeared since this would have resulted in changing a six-parent to a five-parent half-diallel.

Tests having only subsets of the half-sib families present in common are a frequent occurrence in data analysis at CFGRP. This partial connectedness was simulated by generating data in which only 10 of the 15 families present in a test were common to either one of the other two tests comprising a data set.

Variance component estimation techniques

Two algorithms were utilized for all estimation techniques: sequentially adjusted sums of squares (Milliken and Johnson 1984, p 138) for HM3; and Giesbrecht's algorithm (Giesbrecht 1983) for REML, ML, MINQUE and MIVQUE. Giesbrecht's algorithm is primarily a gradient algorithm (the method of scoring), and as such allows negative estimates (Harville 1977; Giesbrecht 1983). Negative estimates are not a theoretical difficulty with MINQUE or MIVQUE; however, for REML and ML, estimates should be confined to the parameter space. For this reason estimators referred to as REML and ML in this paper are not truly REML and ML when negative estimates occur; further, there is the possibility that the iterative solution stopped at local maxima and not at the global maximum. These concerns are commonplace in REML and ML estimation (Corbeil and Searle 1976; Harville 1977; Swallow and Monahan 1984); however, ignoring these two points, these estimators are still referred to as REML and ML.

The basic equation under normality (Giesbrecht 1983) for MIVQUE, MINQUE and REML is

$$\underset{rxr\,rx1}{[\mathrm{tr}(\mathbf{QV}_i\mathbf{QV}_j)]}\,\hat{\sigma}^2 = \underset{rx1}{[y'\mathbf{QV}_i\mathbf{Qy}]} \tag{8}$$

then

$$\hat{\sigma}^2 = [\mathrm{tr}(\mathbf{QV}_i\mathbf{QV}_j)]^{-1}[\mathbf{y}'\mathbf{QV}_i\mathbf{Qy}];$$

and for ML

$$\underset{rxr}{[\mathrm{tr}(\mathbf{V}^{-1}\mathbf{V}_i\mathbf{V}^{-1}\mathbf{V}_j)]}\,\underset{rx1}{\hat{\sigma}^2} = \underset{rx1}{[\mathbf{y}'\mathbf{QV}_i\mathbf{Qy}]}; \tag{9}$$

where (a_{ij}) is a matrix whose elements are a_{ij} where in the full-sib designs $i = 1$ to 8 and $j = 1$ to 8, that is there is a row and column for every random variable in the linear model;
tr is the trace operator, that is the sum of the diagonal elements of a matrix;
$\mathbf{Q} = \mathbf{V}^{-1} - \mathbf{V}^{-1}\mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})\mathbf{X}'\mathbf{V}^{-1}$ for $\mathbf{V}$ as the dispersion matrix of $\mathbf{y}$ and $\mathbf{X}$ as the design matrix for fixed effects;
$\mathbf{V}_i = \mathbf{Z}_i\mathbf{Z}_i'$ where $\mathbf{i}$ = the random variables test, block, etc.;
$\hat{\boldsymbol{\sigma}}^2$ is the vector of variance component estimates; and
$\mathbf{r}$ is the number of random variables in the model.

The MINQUE estimator used was MINQUE1, i.e., with ones as priors for all variance components; calculated by applying the Giesbrecht's algorithm non-iteratively. MINQUE1 was chosen because of results demonstrating MINQUE0 (prior of 1 for the error term and of 0 for all others) to be an inferior estimation technique for many cases (Swallow and Monahan 1984; R. C. Littell, unpublished data).

With normally distributed uncorrelated random variables, the use of the true values of the variance components as priors in a non-iterative application of Giesbrecht's algorithm produced the MIVQUE solutions (equation 8). Obtaining true MIVQUE estimation is a luxury of computer simulation and would not be possible in practice since the true variance components are required (Swallow and Searle 1978). This estimator was included to provide a standard of comparison for other estimators. An additional MIVQUE-type estimator, referred to as MIVPEN, was also included. MIVPEN too was a non-iterative application of the algorithm with the true variance components as priors; however, this estimator was conditioned on the variance component parameter space and did not allow negative estimates. The non-negative conditioning of MIVPEN was accomplished by adding a penalty algorithm to MIVQUE such that no variance component was allowed to be less than 1×10^{-7}. The penalty algorithm operated by using $\Delta = \hat{\sigma}^2 - \sigma^2$ and by choosing a scalar weight w such that no element of $\hat{\sigma}^2_{\text{new}}$ is less than 1×10^{-7}. Then $\hat{\sigma}^2_{\text{new}} = \sigma^2 + w\Delta$, where Δ is the vector of departure from the true values (σ^2), 1×10^{-7} is an arbitrary constant and $\hat{\sigma}^2_{\text{new}}$ is the vector of estimated variance components conditioned on non-negativity.

REML estimates were from repeated application of Giesbrecht's algorithm (equation 8) in which the estimates from the k-th iteration become the priors for the $k+1$-th iteration. The iterations were stopped when the difference between the estimates from the k-th and $k+1$-th iterations met the convergence criterion; then the estimates of the $k+1$-th iteration became the REML estimates. The convergence criterion utilized was $\sum_{i=1}^{r}|\hat{\sigma}^2_{i(k)} - \hat{\sigma}^2_{i(k+1)}| < 1 \times 10^{-4}$. This criterion imposed convergence to the fourth decimal place for all variance components. The robustness of REML solutions obtained from Giesbrecht's algorithm to priors (or starting points) was explored. The difference in solutions starting from two distinct points (a vector of ones or the true values) was compared over 2 000 data sets of different structures (imbalance, true variance components, and field design). The results (agreeing with those of Swallow and Monahan 1984) indicated that the difference between the two solutions was entirely dependent on the stringency of the convergence criterion and not on the starting point (priors). Thus, all REML estimates were calculated starting with the true values as priors.

Three alternatives for coping with negative estimates after convergence were used for REML solutions: accept and use the negative estimates (Shaw 1987), arbitrarily set negative estimates to zero, and re-solve the system setting negative estimates to zero (Miller 1973). The first two alternatives are self-explanatory and the latter is accomplished by re-analyzing those data sets in which the initial unrestricted REML estimates included one or more negative estimates. During re-analysis if a variance component became negative, it was set to zero (could never be any value other than zero) and the iterations continued. This procedure persisted until the convergence criterion was met with a solution in which all variance components were either positive or zero.

ML solutions, as iterative applications of equation 9, were calculated from the same starting points and with the same convergence criterion as REML solutions. The same alternatives for negative variance components were explored for ML as for REML.

The algorithm to calculate solutions for HM3 (sequentially adjusted sums of squares) was based on the upper triangular G2 sweep (Goodnight 1979) and Hartley's method of synthesis (Hartley 1967). The equation solved was $E(\mathbf{MS})\hat{\sigma}^2 = \mathbf{MS}$ where $\mathbf{MS}$ is the vector of mean squares and $E(\mathbf{MS})$ is their expectation. The alternative used for negative estimates was to ignore the fact that they were negative.

Comparison among estimation techniques

For the simulation MIVQUE estimates were the basis for all comparisons because MIVQUE is by definition the minimum variance quadratic unbiased estimator. The results of comparing the mean of 1 000 MIVQUE estimates for an experimental level to the means for other techniques were termed "apparent bias". "Apparent bias" denotes that 1 000 data sets were not sufficient to achieve complete convergence to the true values of the variance components.

Sampling variances of estimation were calculated from the 1 000 observations within an experimental level and estimation technique for variance components and genetic ratios (single tree heritability, Type B correlation and dominance to additive variance ratio) Mean square error then equalled variance plus squared "apparent bias". While mean square error was investigated, there was never sufficient bias for mean square error to lead to a different decision concerning techniques than that obtained with the sampling variance of the estimates; so mean square error was deleted from the remainder of this discussion.

Probability of nearness is the probability that an estimate will lie within a certain interval around the true parameter. The three total interval widths utilized were one-half, equal to, and twice the parameter size. The percentage of 1 000 estimates falling within these intervals was calculated for the different estimation techniques within an experimental level for both variance components and ratios and utilized as an estimate of probability of nearness.

Results are presented by variance component or genetic ratio estimated as a percentage of MIVQUE (except in the case of probability of nearness). MIVQUE estimates represent 100%, with estimates with greater variance having values larger than 100% and "apparently biased" estimates having values different from 100%. For probability of nearness, larger percentages (probabilities) are favored since they are indicative of greater density of estimates near the parametric value.

Results and discussion

Variance components

Sampling variance of the estimators. For all variance components estimated (Table 2), REML and ML were consistently equal to or less than MIVQUE for sampling the variance of the estimator. The variance among estimates from these techniques was further reduced by setting the negative components to zero (MODML and MODREML) or setting negative estimates to zero plus re-solving the system (NNREML, NNML, and PNNREML). MINQUE1 sampling variance is always equal to or greater than MIVQUE, as one might expect, since they are, in this application, the same technique with MIVQUE having perfect priors. Variance for HM3 estimators (TYPE3 and PTYPE3) is either equal to or greater than MIVQUE with the extent of the departure dependent on the level of imbalance. MIVPEN, although not practical, had much more precise estimates of variance components than other techniques, illustrating what could be accomplished given the true values as priors plus maintaining estimates within the parameter space.

An analysis of variance was conducted to determine the importance of the treatment of negative variance component estimates in the variance of estimation for REML and ML estimates. The model of sampling variance of the estimates as a result of mating design, imbalance level, treatment of negative estimates and size of the variance component, demonstrated consistently (for all variance components except error) that treatment of negative estimates is an important component of the variance of the estimates ($P < 0.05$). The model accounted for up to 99% (σ_g^2 of the variation in the variance of the variance component estimates with: (1) accepting and using negative estimates producing the highest variance; (2) setting the negative components to zero being intermediate; and (3) re-solving the system with negative estimates set to zero providing the lowest variance.

For all estimation techniques, lower variance among estimates was obtained by using individual observations as compared to plot means. The advantage of individual over plot-mean observations increased with increasing imbalance.

Bias. The most consistent performer for bias (Table 3) was TYPE3, known from inherent properties to be unbiased. The consistent convergence of the TYPE3 value to the MIVQUE value indicated that the number of data sets used (1 000 per technique and experimental level) was suitable for the purpose of examining bias. The other two consistent performers were REML and MINQUE1. Bias resulted primarily from the method of dealing with negative estimates.

Probability of nearness. Results for probability of nearness proved to be largely non-discriminatory among techniques (Table 3). The low levels of probability density near the parametric values is indicative of the nature of the variance component estimation problem.

Table 2 Abbreviation for and description of variance component estimation methods utilized for analyses based on individual observations (if utilized for plot-mean analysis the abbreviation is modified by pre-fixing a '*P*')

Abbreviation	Description	Citation
ML PML	Maximum likelihood: estimates not restricted to the parameter space (individual and plot-mean analysis).	Hartley and Rao 1967; Shaw 1987
MODML	Maximum likelihood: negative estimates set to zero after convergence (individual analysis)	Hartley and Rao 1967
NNML	Maximum likelihood: if negative estimates appeared at convergence, they were set to zero and the system re-solved (individual analysis)	Hartely and Rao 1967; Miller 1973
REML PREML	Restricted maximum likelihood: estimates not restricted to the parameter space (individual and plot-mean analysis)	Patterson and Thompson 1971; Shaw 1987; Harville 1977
MODREML	Restricted maximum likelihood: negative estimates set to zero after convergence (individual analysis)	Patterson and Thompson 1971
NNREML PNNREML	Restricted maximum likelihood: if negative estimates appeared at convergence, they were set to zero and the system re-solved (individual and plot-mean analysis)	Patterson and Thompson 1971; Miller 1983
MIVQUE PMIVQUE	Minimum variance quadratic unbiased: non-interative with true (parametric) values of the variance components as priors (individual and plot-mean analysis)	Rao 1971b
MINQUE1 PMINQUE1	Minimum norm quadratic unbiased: non-interative with ones as priors for all variance components (individual and plot-mean analysis)	Rao 1971a
TYPE3 PTYPE3	Sequentially adjusted sums of squares; Henderson's Method 3 (individual and plot-mean analysis)	Henderson 1953
MIVPEN	MIVQUE with a penalty algorithm to prevent negative estimates (individual analysis)	Harville 1977

Table 3 Sampling variance of the estimates (left column, as a percentage of the MIVQUE estimate), Bias (center column, as a percentage of the MIVQUE estimate) and Probability of nearness (interval equals the parameter magnitude, as percentage of estimates in the interval) for σ_g^2 (upper row), σ_{tg}^2 (second row), and h^2 (third row where calculated) within each cell by type of estimator and treatment combination. NA is not applied

Estimator	D1S80	D1S65	D2S65	H1S80	H1S65
REML	100 100 33	103 102 24	102 99 42	100 100 45	106 103 29
	100 100 43	100 102 26	104 100 26	100 100 37	98 99 27
	100 100 34	101 101 25	101 99 45	100 100 45	106 103 28
ML	77 75 34	78 62 22	76 76 41	96 96 45	104 98 29
	107 107 43	105 115 26	111 110 25	101 101 36	99 102 27
	82 76 35	83 62 22	86 78 45	96 96 46	104 98 28
MINQUE1	100 100 33	104 96 25	104 99 41	104 99 45	147 102 26
	101 100 43	119 101 24	124 101 25	112 101 34	140 98 23
	100 100 34	106 97 25	104 99 45	104 99 45	146 101 26
NNREML	81 108 33	72 116 23	95 98 42	88102 45	69 108 29
	68 93 45	48 92 28	55 93 26	79 100 38	49 102 29
	77 109 34	64 118 24	92 98 46	87 102 45	68 108 30
NNML	NA	NA	NA	83 102 50	65 108 30
				79 100 38	49 102 29
				83 98 46	65 104 29
MODML	58 87 34	50 90 22	70 79 41	85 98 45	75 114 29
	13 110 43	82 130 26	82 127 25	87 101 36	68 123 27
	58 88 35	46 92 22	72 79 45	84 100 46	71 113 28
MODREML	82 110 33	74 124 24	96 101 42	89 103 45	78 118 29
	89 104 43	74 120 26	74 119 26	85 105 37	67 121 27
	76 110 34	64 123 25	89 98 45	88 103 45	74 116 28
TYPE3	101 100 34	101 99 23	106 100 42	101 100 45	121 100 27
	101 100 43	101 101 27	116 102 25	101 100 37	126 101 25
	100 100 35	108 100 24	103 99 46	100 100 46	122 100 27
PREML	100 100 32	106 99 20	102 98 42	108 100 44	147 111 25
	103 100 43	114 104 27	120 100 25	122 102 32	151 98 20
PML	78 74 34	82 58 20	77 74 40	104 96 44	143 105 24
	110 107 41	117 116 26	127 112 24	123 103 32	152 102 21
PMINQUE1	100 100 32	108 95 21	105 99 40	108 100 44	179 106 24
	103 100 43	129 102 25	137 103 23	122 102 32	181 115 22
PNNREML	81 108 32	71 114 19	94 97 41	93 102 43	87 116 26
	70 93 43	53 94 28	60 95 23	94 104 33	68 110 21
PTYPE3	100 100 32	107 97 23	105 99 42	108 100 44	168 104 25
	103 100 43	125 97 25	133 96 24	122 102 32	185 109 22
	101 100 33	111 98 24	104 99 46	107 100 45	168 104 25
MIVPEN	NA	36 107 41	29 99 78	80 102 48	46 103 36
		27 99 47	20 92 60	74 101 39	40 105 31
		35 113 42	30 104 80	80 102 49	45 103 35
PMIVQUE	100 100 32	104 97 20	102 99 42	108 100 44	147 107 26
	103 100 43	114 102 28	118 100 27	122 102 32	151 99 21

Ratios of variance components

Single tree heritability. Results for estimates of single tree heritability adjusted for locations and blocks are shown in Tables 2 and 3 (third number from the top in each cell, if calculated). For these relatively low heritabilities (0.1 and 0.25), the bias and variance properties of the estimated ratio are similar to those for σ_g^2 estimates. This implies that the denominator of the heritability estimate (the phenotypic variance estimate) is relatively stable across techniques and, as the denominator of a ratio with an expected value of 0.1 or 0.25, has little effect on the variance of the ratio (Kendall and Stuart 1963). Variance component estimation techniques which performed well for bias and/or variance among estimates for σ_g^2 also performed well for h^2.

Type B correlation and dominance to additive variance ratio. Type B correlation (refer to σ_{tg}^2 Tables 1 and 3) and dominance to additive variance ratio (data not shown) estimates both proved to be too unstable (extremely large variance among estimates) to be useful in discrimination among variance component estimation techniques. This high variance is due to the estimates of the denominators of these ratios approaching zero and to the high variance of the denominator of ratios (Tables 1 and 3).

Recommendation

If one were to choose a single variance component estimation technique from among those tested which could be applied to any data set with confidence that the estimates had desirable properties (variance, MSE, and bias), that technique would be REML and the basic unit of analysis would be the individual observation. This combination (REML plus individual observations) performed well across mating design and types and levels of imbalance. Treatment of negative estimates would be determined by the use of the estimates; that is, whether unbiasedness (accepting and using the negative estimates) is more important than sampling variance (re-solve the system setting negative estimates to zero).

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