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Evaluation of variance component estimators based on Henderson's Method

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Abstract

A two-way linear mixed model consisting of three variance components, σ_1^2, σ_2^2 and σ_e^2 is applied to evaluate the performance of the modified variance component estimator obtained from Henderson's (1953) method 3, developed by Al-Sarraj and von Rosen (2009). The estimator of interest σ_1^2, is obtained and modified, from two different partitions, (partition I and partition II), of the Henderson's method 3 equations. By means of simulation, we evaluate the performance of these variance component estimators. The evaluation is in terms of mean square errors, estimated biases and probability of obtaining negative estimates. In addition, the comparison includes also variance component estimators obtained from likelihood-based procedures, REML and ML. The effect of imbalance and number of observations on mean square error is given. The modified Henderson's method 3 variance component estimator obtained from partition I is recommended for values of $\sigma_2^2/\sigma_1^2 < 1.0$. In terms of mean square errors and probability of obtaining negative estimates, the modified Henderson's method 3 has achieved improvement over the corresponding non-modified ones. Further, unlike the likelihood-based estimators, the modified variance component estimators are non-iterative, and therefore computationally faster, with similar performance in terms of mean square error as the ML estimator.

Keywords: Variance components, ML, REML, Henderson's method 3

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1 Introduction

Variance component estimation has a wide application in various fields of science e.g. it is often used in population genetics and applied animal breeding. There are several estimation methods found in the literature (see e.g. Searle, Casella & McCulloch (1992)), bearing in mind each of those methods has its own advantages and disadvantages.

The most commonly used methods are the ANOVA method, the Minimum Quadratic Unbiased Estimator (MINQUE) and the Minimum Variance Quadratic Unbiased Estimator (MIVQUE) by Rao (1971a, 1971b, 1972), the likelihood-based procedures (the Maximum likelihood estimator (ML) and the Restricted Maximum Likelihood Estimator (REML) by Hartley and Rao (1967) and Patterson and Thompson (1971) respectively). The obtained ML and REML estimators have good statistical properties. They are functions of the sufficient statistics, are consistent, asymptotically normal, and further, the asymptotic sampling dispersion matrix of the estimators is known. However, these likelihood-based procedures are computationally demanding, and an extensive review of the procedures has been presented by Harville (1977).

Henderson (1953) presented the non-iterative ANOVA-like methods that give rise to unbiased variance component estimators. The methods are known as Henderson's method 1, 2 and 3; each of which is suitable for a certain situation. Method 3 is the most general one, it allows for fixed, random and interaction effects in the model. However, the obtained estimators can assume negative values; a fact that renders them inferior to the ones obtained by the likelihood-based procedures. Therefore, an attempt was made to improve the unbiased variance component estimator obtained from applying Henderson's method 3 in a two-way linear mixed model (see Al-Sarraj & von Rosen (2009)). Further, the modified variance component estimator was shown to perform better in terms of mean square error criteria under certain conditions.

Rönnegård *et al* (2009) tested the utility of the modified Henderson's method 3 estimator in a Quantitative Trait Loci (QTL) study as an alternative method for the likelihood-based procedures commonly used in this particular field.

The aim of the current study is to compare and evaluate the performance of the modified estimators (obtained by Al-Sarraj and von Rosen (2009) from two different decompositions/partitions of Henderson's method 3) with the non-modified variance component estimator. Further these estimators were compared to ML and REML estimators. The comparison was performed in terms of mean square error (MSE), estimated biases, and the probability of getting negative variance estimates.

2 Material and methods

2.1 Two-way linear mixed model

The considered model is a two-way linear mixed model:

$$Y = X\beta + Z_1 u_1 + Z_2 u_2 + e, \tag{2.1}$$

where Y is an $n \times 1$ vector of observations distributed as a multivariate normal MVN $(X\beta, V)$, $X : n \times m$ the design or incidence matrix of known elements, $\beta : m \times 1$ a vector of unknown fixed effect parameters and $e : n \times 1$ a vector representing the within-subject variability or the measurement error distributed as $e \sim MVN(0, \sigma_e^2 I)$, where I is the $n \times n$ identity matrix. The first random effect of (2.1) u_1 is a $p \times 1$ vector normally distributed $u_1 \sim MVN(0, \sigma_1^2 I)$, whereas the second random effect is represented by u_2 a $q \times 1$ normally distributed vector $u_2 \sim MVN(0, \sigma_2^2 I)$. Further, $Z_1 : n \times p$ and $Z_2 : n \times q$ are known incidence matrices, $V = \sigma_1^2 V_1 + \sigma_2^2 V_2 + \sigma_e^2 I$ is the dispersion matrix and $V_1 = Z_1 Z_1'$ and $V_2 = Z_2 Z_2'$ are known design matrices. The variance components in (2.1) are σ_1^2, σ_2^2 and σ_e^2; the first two correspond to the first and second random effect, whereas the third is the variance of the error component.

2.2 Modified Henderson's method 3

Henderson's method 3 was one of the three methods Henderson developed in 1953, which dealt with the deficiencies of Henderson method 1 and 2, for details see Searle, Casella and McCulloch (1992). The modified version is based on Henderson's method 3 equations, but relaxes the condition of unbiasedness. Henderson's method 3 is applied on a two-way linear mixed model (2.1), where two decompositions of the equations are studied referred to as partition I and partition II.

In partition I, three variance components are included; σ_1^2, σ_2^2 and σ_e^2 whereas, only two variance components are included in partition II; σ_1^2 and σ_e^2 where σ_2^2 is eliminated by an orthogonal projection. In both partitions, the work was focused on σ_1^2.

For the two partitions, this variance component estimator was improved by perturbing the standard unbiased estimator so that the obtained estimator would have a mean square error that is less than the non-modified one, for details see Al-Sarraj and von Rosen (2009), Kelly and Mathew (1994). The variance component estimators resulting from partition I and II are denoted $\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,u_2}$ respectively, whereas their corresponding modified estimators are denoted $\widehat{\sigma}^2_{1,m_1}$ and $\widehat{\sigma}^2_{1,m_2}$ respectively. All four variance component estimators are given in Appendix A.

2.3 Measure of imbalance

In unbalanced data the number of observations at each level of the random effect is different, and a measure is needed to quantify the imbalance. In (2.1), the number of observation n_i defines the structure of the data at different levels of the random effects. Ahrens and Pincus (1981) proposed several measures of imbalance which under certain transformations are identical, one of which is

$$v_m(n) = \frac{1}{m \sum (\frac{n_i}{n})^2}, \tag{2.2}$$

where $n = \sum_i n_i$, $m = p$ (or q) and $i = 1, \cdots p$ (or $1, \cdots q$). In unbalanced data the value of $v_m(n)$ is within the range $\frac{1}{m} \leq v_m(n) < 1$; so the smaller the $v_m(n)$ value is the more imbalanced the data are. The maximum value of $v_m(n) = 1$ occurs only when the data are balanced. For a two-way linear mixed model (2.1), $v_p(n)$ and $v_q(n)$ denote the imbalance for the design matrices Z_1 and Z_2 respectively. Here, the following measure is suggested to calculate the imbalance in the considered examples, given in Appendix C,

$$v(n) = 0.5 v_p(n) + 0.5 v_q(n).$$

2.4 Monte Carlo comparisons and simulations

The variance component estimators resulting from applying the different methods of estimation are compared in the context of different patterns of data and true values of the variance components. Swallow and Monahan (1984) illustrated that the subgroup means and subgroup sums of squares are sufficient for the variance component estimators. This was exploited in our Monte Carlo simulation by using a modified polar method (Marsglia and Bray, 1964) for generating normal random variables. Six different examples given in Appendix C which were also considered by Al-Sarraj and von Rosen (2009), are used. Following subsection 2.3, the degree of imbalance was calculated for these six examples, see Table 1.

The value of $v(n)$ shows the following: Example 1 is a balanced case, whereas, Examples 2 and 4 are almost balanced. The remaining Examples 3, 5 and 6 are more unbalanced than the others.

In the following subsections, we compare the different estimators based on Henderson's method with ML and REML. The MSE, estimated bias and probability of getting negative estimates for these estimators are investigated in five different case studies:

Table 1: The imbalance measure for each example

Example	n	p	q	$v_p(n)$	$v_q(n)$	$v(n)$
1	8	2	2	1	1	1
2	8	2	2	0.9412	0.9412	0.9412
3	8	2	2	0.8000	0.9412	0.8706
4	21	3	3	0.9439	0.9866	0.9653
5	30	3	3	0.8571	0.7937	0.8254
6	30	4	3	0.8858	0.8772	0.8815

Case 1: The impact of varying σ_2^2 for a given value of σ_1^2 on the MSE.
Case 2: The impact of varying σ_1^2 for a given value of σ_2^2 on the MSE.
Case 3: Probability of obtaining negative estimates.
Case 4: The choice of partition (I or II) depending on the ratio σ_2^2/σ_1^2.
Case 5: The influence of the number of observations on the MSE.

For each simulation 1000 replicates were used. For the ML and REML estimates, the lmer() function in the lme4 R package (Bates and Maechler, 2010) was used.

2.4.1 Case 1: The impact of varying σ_2^2 for a given value of σ_1^2 on the MSE

The main idea behind modifying the variance component estimators for the two considered partitions was to obtain an estimator that would perform better in terms of MSE criteria. Thus, for partition I and II, the MSE($\widehat{\sigma}^2_{1,u_1}$) should be less than MSE($\widehat{\sigma}^2_{1,u_2}$), likewise their modified corresponding estimators MSE($\widehat{\sigma}^2_{1,m_1}$) less than MSE($\widehat{\sigma}^2_{1,m_2}$) and for this to be achieved there are a range of values for σ_2^2. Therefore, we chose ten different values of $\sigma_2^2 = 0.01, 0.05, 0.1, 0.15, 0.25, 0.5, 0.75, 1, 1.5, 2$ for calculation of the MSEs of the variance component estimators $\widehat{\sigma}^2_{1,u_1}$, $\widehat{\sigma}^2_{1,u_2}$, $\widehat{\sigma}^2_{1,m_1}$ and $\widehat{\sigma}^2_{1,m_2}$ that would thereafter be compared. The true values for the other parameters, used in the simulation, were $\mu = 0$, $\sigma_1^2 = 0.1$, $\sigma_e^2 = 0.9$. The equations used to estimate $\widehat{\sigma}^2_{1,u_1}$, $\widehat{\sigma}^2_{1,u_2}$, $\widehat{\sigma}^2_{1,m_1}$ and $\widehat{\sigma}^2_{1,m_2}$ are given in (A.1),(A.3),(A.2) and (A.4) respectively. The observed MSEs of the variance component estimators were calculated as in Appendix D and the MSEs of the variance component estimators obtained from the two considered partitions (I and II) is given in Appendix B. For further details and calculations of the MSEs see (Al-Sarraj & von Rosen, 2009).

2.4.2 Case 2: The impact of varying σ_1^2 for a given value of σ_2^2 on the MSE

As the MSEs of $\widehat{\sigma}_{1,u_1}^2$ and $\widehat{\sigma}_{1,m_1}^2$ depend among others on σ_1^2, in this analysis we chose one value from the range of $\sigma_2^2 < 0.1$ based on Case 1 with 10 different values of $\sigma_1^2 = 0.001, 0.01, 0.05, 0.10, 0.15, 0.20, 0.5, 1.0, 2.0, 5.0$. For the simulation, the true values of $\mu = 0$ and $\sigma_e^2 = 0.9$ were applied, and from the range of σ_2^2, 0.05 was chosen. Moreover, the MSEs of the variance component estimators $\widehat{\sigma}_{1,u_1}^2$, $\widehat{\sigma}_{1,m_1}^2$, $\widehat{\sigma}_{1,u_2}^2$ and $\widehat{\sigma}_{1,m_2}^2$ were compared, and further the comparison included variance component estimators obtained by the commonly used methods $\widehat{\sigma}_{1,ML}^2$ and $\widehat{\sigma}_{1,REML}^2$. Besides, for the ten different values of σ_1^2, the estimated biases for all the examples were calculated.

2.4.3 Case 3: Probability of obtaining negative estimates for the two partitions

For all the six examples including both partitions (I and II) and their modified corresponding estimators, the probability of obtaining negative estimates was determined, see Appendix D.

2.4.4 Case 4: The choice of partition (I or II) based on the ratio σ_2^2/σ_1^2

Based on the results from Case 1 and Case 2, for MSE($\widehat{\sigma}_{1,u_1}^2$) and MSE($\widehat{\sigma}_{1,m_1}^2$) to be smaller than MSE($\widehat{\sigma}_{1,u_2}^2$) and MSE($\widehat{\sigma}_{1,m_2}^2$), respectively, a value range for $\sigma_2^2 < 0.1$ was recommended. However, since the true values of the variance components may vary within a wide range, there was a need to extend $\sigma_2^2 < 0.1$ for wider application purposes and consequently the ratio σ_2^2/σ_1^2 was considered. Based on the same calculation mentioned above, the ratio $\sigma_2^2/\sigma_1^2 < 1$ was applied and from which $\sigma_2^2/\sigma_1^2 = 0.8$ was chosen; a ratio that could be obtained from many different values of σ_2^2 and σ_1^2. For the simulation we applied the following variance components' values $\sigma_2^2 = 0.8, 4, 12, 24, 40, 80$ and $\sigma_1^2 = 1, 5, 15, 30, 50, 100$. Hence, the range of σ_2^2 and σ_1^2 could cover many true values in real experiments. For the other parameters in the model, the values $\mu = 0$ and $\sigma_e^2 = 0.9$ were applied. For Examples 2 and 5, the same above mentioned ratio was tested and the MSEs of $\widehat{\sigma}_{1,u_1}^2$, $\widehat{\sigma}_{1,u_2}^2$, $\widehat{\sigma}_{1,m_1}^2$ and $\widehat{\sigma}_{1,m_2}^2$ were obtained.

2.4.5 Case 5: The influence of the number of observations on the MSE

The main task here, was to see what impact n would have on the MSEs of the different variance component estimators. For the simulation, $\sigma_1^2 = 1$, $\sigma_2^2 = 0.05$, $\sigma_e^2 = 0.9$ and $\mu = 0$ were used. The MSEs of $\widehat{\sigma}^2_{1,u_1}$, $\widehat{\sigma}^2_{1,m_1}$ and $\widehat{\sigma}^2_{1,ML}$ were calculated. Example 5, being most unbalanced, was applied as the basic experiment. Four different $n = 30, 150, 450, 900$ were used, and thereafter MSEs were calculated for the different values of n.

3 Results

3.1 Case 1: The impact of varying σ_2^2 for a given value of σ_1^2 on the MSE

Example 1 is a balanced case and the MSEs of $\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,u_2}$ were therefore equal (Table 2). This was also the case for $\widehat{\sigma}^2_{1,m_1}$ and $\widehat{\sigma}^2_{1,m_2}$ (Table 3). Furthermore, in Example 2, the MSE of $\widehat{\sigma}^2_{1,u_1}$ was similar to those of $\widehat{\sigma}^2_{1,u_2}$ since Example 2 is close to balanced. In Example 4, the MSE($\widehat{\sigma}^2_{1,u_1}$) was smaller than MSE($\widehat{\sigma}^2_{1,u_2}$) when σ_2^2 was small. Meanwhile, when the value of σ_2^2 was large the MSE increased dramatically. For Examples 3, 5 and 6, both MSE of $\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,m_1}$ showed a successively rising trend as σ_2^2 increased. Since the MSEs of $\widehat{\sigma}^2_{1,u_2}$ and $\widehat{\sigma}^2_{1,m_2}$ are independent of σ_2^2 by definition, their observed MSEs remained unchanged. The MSE of all four estimators benefited from larger n as expected.

Moreover, for a fixed $\sigma_1^2 = 0.1$ and changes in σ_2^2, both $\widehat{\sigma}^2_{1,m_1}$ and $\widehat{\sigma}^2_{1,m_2}$ were improved substantially in comparison to the non-modified variance component estimators $\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,u_2}$ in terms of MSE.

In the last columns of Tables 2 and 3 the range of values of σ_2^2 is given where the MSEs of $\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,m_1}$ were found to be less than the MSEs for $\widehat{\sigma}^2_{1,u_2}$ and $\widehat{\sigma}^2_{1,m_2}$, respectively. Based on the results from Table 2 and Table 3, partition I is recommended for $\sigma_2^2 < 0.1$ in all the unbalanced examples considered.

3.2 Case 2: The impact of varying σ_1^2 for a given value of σ_2^2 on the MSE

The observed MSEs of $\widehat{\sigma}^2_{1,u_1}$ were lower than $\widehat{\sigma}^2_{1,u_2}$ except in Example 1 and Example 2 (Table 4). Partition I showed lower MSEs than partition II for

Table 2: The observed MSE of $\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,u_2}$ based on 10 different σ_2^2, $\mu = 0$, $\sigma_1^2 = 0.1$ and $\sigma_e^2 = 0.9$ with $N = 1000$ simulations

		σ_2^2										
Ex	est.	0.01	0.05	0.1	0.15	0.25	0.5	0.75	1	1.5	2	σ_2^2
1	$\widehat{\sigma}^2_{1,u_1}$	0.2351	0.2399	0.2453	0.2053	0.2129	0.2051	0.2417	0.2209	0.2340	0.2254	None
	$\widehat{\sigma}^2_{1,u_2}$	0.2351	0.2399	0.2453	0.2053	0.2129	0.2051	0.2417	0.2209	0.2340	0.2254	
2	$\widehat{\sigma}^2_{1,u_1}$	0.2759	0.2420	0.2785	0.2575	0.2574	0.2429	0.2622	0.2462	0.2710	0.2693	$\sigma_2^2 < 0.15$
	$\widehat{\sigma}^2_{1,u_2}$	0.2755	0.2440	0.2845	0.2604	0.2524	0.2423	0.2579	0.2463	0.2643	0.2583	
3	$\widehat{\sigma}^2_{1,u_1}$	0.4255	0.3340	0.3626	0.3556	0.4291	0.3418	0.3962	0.3467	0.4597	0.4496	$\sigma_2^2 < 0.15$
	$\widehat{\sigma}^2_{1,u_2}$	0.4343	0.3418	0.3802	0.3552	0.4510	0.3359	0.3726	0.3159	0.3683	0.4073	
4	$\widehat{\sigma}^2_{1,u_1}$	0.0805	0.0918	0.1103	0.1246	0.1653	0.4000	0.5294	0.9613	1.4926	3.0523	$\sigma_2^2 < 0.25$
	$\widehat{\sigma}^2_{1,u_2}$	0.1498	0.1876	0.1452	0.1364	0.1418	0.1480	0.1306	0.1536	0.1463	0.1424	
5	$\widehat{\sigma}^2_{1,u_1}$	0.04558	0.0447	0.0471	0.0499	0.0635	0.0952	0.1336	0.1977	0.3163	0.4955	$\sigma_2^2 < 0.25$
	$\widehat{\sigma}^2_{1,u_2}$	0.0635	0.0568	0.0644	0.0541	0.0562	0.0603	0.0585	0.0587	0.0553	0.0589	
6	$\widehat{\sigma}^2_{1,u_1}$	0.0413	0.0560	0.0580	0.0673	0.1031	0.1839	0.2575	0.3835	0.5989	0.8223	$\sigma_2^2 < 0.10$
	$\widehat{\sigma}^2_{1,u_2}$	0.0490	0.0575	0.0499	0.0530	0.0560	0.0508	0.0582	0.0527	0.0568	0.0563	

Table 3: The observed MSE of $\widehat{\sigma}^2_{1,m_1}$ and $\widehat{\sigma}^2_{1,m_2}$ based on 10 different σ_2^2, $\mu = 0$, $\sigma_1^2 = 0.1$ and $\sigma_e^2 = 0.9$ with $N = 1000$ simulations

		σ_2^2										
Ex	est.	0.01	0.05	0.1	0.15	0.25	0.5	0.75	1	1.5	2	σ_2^2
1	$\widehat{\sigma}^2_{1,m_1}$	0.0269	0.0277	0.0280	0.0235	0.0249	0.0240	0.0270	0.0256	0.0266	0.0264	None
	$\widehat{\sigma}^2_{1,m_2}$	0.0269	0.0277	0.0280	0.0235	0.0249	0.0240	0.0270	0.0256	0.0266	0.0264	
2	$\widehat{\sigma}^2_{1,m_1}$	0.0312	0.0274	0.0312	0.0288	0.0292	0.0279	0.0292	0.0282	0.0305	0.0309	$\sigma_2^2 < 0.25$
	$\widehat{\sigma}^2_{1,m_2}$	0.0311	0.0276	0.0318	0.0290	0.0287	0.0287	0.0281	0.0297	0.0298		
3	$\widehat{\sigma}^2_{1,m_1}$	0.0464	0.0363	0.0397	0.0392	0.0468	0.0376	0.0430	0.0383	0.0500	0.0495	$\sigma_2^2 < 0.5$
	$\widehat{\sigma}^2_{1,m_2}$	0.0471	0.0370	0.0414	0.0391	0.0491	0.0369	0.0404	0.0352	0.0403	0.0445	
4	$\widehat{\sigma}^2_{1,m_1}$	0.0182	0.0208	0.0236	0.0251	0.0308	0.0745	0.0954	0.1955	0.2844	0.5231	$\sigma_2^2 < 0.25$
	$\widehat{\sigma}^2_{1,m_2}$	0.0277	0.0336	0.0275	0.0258	0.0261	0.0276	0.0246	0.0283	0.0268	0.0264	
5	$\widehat{\sigma}^2_{1,m_1}$	0.0122	0.0120	0.0124	0.0127	0.0149	0.0196	0.0273	0.0340	0.0643	0.0914	$\sigma_2^2 < 0.15$
	$\widehat{\sigma}^2_{1,m_2}$	0.0135	0.0126	0.0138	0.0125	0.0126	0.0133	0.0130	0.0125	0.0125	0.0127	
6	$\widehat{\sigma}^2_{1,m_1}$	0.0137	0.0180	0.0176	0.0191	0.0299	0.0567	0.0821	0.1226	0.2198	0.3137	$\sigma_2^2 < 0.10$
	$\widehat{\sigma}^2_{1,m_2}$	0.0170	0.0196	0.0176	0.0186	0.0189	0.0176	0.0197	0.0181	0.0193	0.0189	

$\sigma_1^2 > 0.01$. Furthermore, the difference in MSEs between the modified and non-modified estimators increased with the value of σ_1^2.

It was also observed that the MSEs of $\widehat{\sigma}^2_{1,ML}$ were smaller than $\widehat{\sigma}^2_{1,REML}$ for all the considered examples. In addition to that, the MSEs of both $\widehat{\sigma}^2_{1,ML}$ and $\widehat{\sigma}^2_{1,m_1}$ were very close and lower than all the other estimators' MSE. Hence, $\widehat{\sigma}^2_{1,ML}$ and $\widehat{\sigma}^2_{1,m_1}$ can be recommended when MSE is concerned.

The estimated biases of $\widehat{\sigma}^2_{1,m_1}$, $\widehat{\sigma}^2_{1,m_2}$ and $\widehat{\sigma}^2_{1,ML}$ increased dramatically, and the results were no longer appealing when σ_1^2 was large (Table 5). Whereas, the biases for the two non-modified estimators ($\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,u_2}$) and $\widehat{\sigma}^2_{REML}$ were more robust and approximately equal to 0. Hence, when unbiasedness is the main concern, the variance component estimators obtained from Henderson's method 3 and REML is recommended.

3.3 Case 3: Probability of obtaining negative estimates for the two partitions

The probability of obtaining negative estimates in all of the examples was similar for both $\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,m_1}$, and likewise for $\widehat{\sigma}^2_{1,u_2}$ and $\widehat{\sigma}^2_{1,m_2}$ (Table 6). It was also observed that the probability of negativity concerning the estimators of both partitions decreased with larger values of σ_1^2. Most importantly, the modified estimators had smaller probability of negativity in comparison with the non-modified ones.

3.4 Case 4: The choice of partition (I or II) depending on the ratio σ_2^2/σ_1^2

In Example 2 which has a low n, the MSEs of $\widehat{\sigma}^2_{1,u_1}$ were larger than the ones for $\widehat{\sigma}^2_{1,u_2}$ apart from a few cases with small differences (Table 7). A similar observation, was made for the MSEs of the modified estimators, i.e., MSE($\widehat{\sigma}^2_{1,m_1}$) was less than MSE($\widehat{\sigma}^2_{1,m_2}$). On the other hand, in Example 5, the MSEs of $\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,m_1}$ were lower than the MSEs of $\widehat{\sigma}^2_{1,u_2}$ and $\widehat{\sigma}^2_{1,m_2}$ respectively. These two examples show that partition I seems to perform better for $\sigma_2^2/\sigma_1^2 < 1.0$. We can conclude that if the MSE is the main interest, the modified estimator $\widehat{\sigma}^2_{1,m_1}$ should be preferred over the other three considered estimators $\widehat{\sigma}^2_{1,u_1}$, $\widehat{\sigma}^2_{1,u_2}$ and $\widehat{\sigma}^2_{1,m_2}$.

Table 4: The observed MSE for estimators of σ_1^2 based on 10 different values of σ_1^2, $\mu = 0$, $\sigma_2^2 = 0.05$ and $\sigma_e^2 = 0.9$ with $N = 1000$ simulations

		σ_1^2									
Ex	est.	0.001	0.01	0.05	0.1	0.15	0.2	0.5	1.0	2.0	5.0
1	$\widehat{\sigma}^2_{1,u_1}$	0.1238	0.1250	0.1719	0.2427	0.3205	0.3607	1.1263	3.1653	9.5649	56.0616
	$\widehat{\sigma}^2_{1,m_1}$	0.0132	0.0128	0.0184	0.0282	0.0295	0.0512	0.2252	0.7693	2.8261	17.4888
	$\widehat{\sigma}^2_{1,REML}$	0.0941	0.0890	0.1351	0.1990	0.2704	0.2997	1.0359	3.0396	9.4204	55.7817
	$\widehat{\sigma}^2_{1,ML}$	0.0175	0.0171	0.0258	0.0404	0.0586	0.0731	0.3109	1.0109	3.4654	20.7649
2	$\widehat{\sigma}^2_{1,u_1}$	0.1658	0.1287	0.2179	0.2562	0.4086	0.4303	1.1886	3.2356	10.0367	50.6879
	$\widehat{\sigma}^2_{1,u_2}$	0.1699	0.1316	0.2153	0.2568	0.4080	0.4292	1.1969	3.2513	10.0444	50.5883
	$\widehat{\sigma}^2_{1,m_1}$	0.0177	0.0130	0.0229	0.0298	0.0483	0.0583	0.2227	0.7667	2.9140	16.9085
	$\widehat{\sigma}^2_{1,m_2}$	0.0182	0.0133	0.0227	0.0298	0.0483	0.0581	0.2230	0.7680	2.9151	16.9052
	$\widehat{\sigma}^2_{1,REML}$	0.1310	0.0869	0.1728	0.2017	0.3448	0.3707	1.1007	3.1020	9.8299	50.3896
	$\widehat{\sigma}^2_{1,ML}$	0.0258	0.0153	0.0339	0.0420	0.0758	0.0882	0.3144	1.0235	3.6079	19.3853
3	$\widehat{\sigma}^2_{1,u_1}$	0.2285	0.1931	0.2795	0.3333	0.4257	0.5784	1.5486	3.1368	9.9593	48.1104
	$\widehat{\sigma}^2_{1,u_2}$	0.2397	0.2119	0.2935	0.3481	0.4611	0.5929	1.5282	3.1542	10.2051	48.4232
	$\widehat{\sigma}^2_{1,m_1}$	0.0243	0.0202	0.0292	0.0368	0.0512	0.0719	0.2515	0.7696	2.8263	16.7087
	$\widehat{\sigma}^2_{1,m_2}$	0.0253	0.0220	0.0305	0.0381	0.0545	0.0728	0.2496	0.7686	2.8419	16.7021
	$\widehat{\sigma}^2_{1,REML}$	0.1771	0.1476	0.2190	0.2598	0.3599	0.4822	1.4154	2.9606	9.8117	47.6020
	$\widehat{\sigma}^2_{1,ML}$	0.0340	0.0247	0.0381	0.0493	0.0739	0.1044	0.3842	1.0216	3.5289	18.9133
4	$\widehat{\sigma}^2_{1,u_1}$	0.0478	0.0465	0.0702	0.0747	0.1059	0.1335	0.4492	1.3921	4.6656	27.0626
	$\widehat{\sigma}^2_{1,u_2}$	0.0710	0.0814	0.1140	0.1372	0.1829	0.2516	0.6670	2.1822	6.9807	34.7800
	$\widehat{\sigma}^2_{1,m_1}$	0.0077	0.0078	0.0137	0.0165	0.0276	0.0380	0.1646	0.5949	2.1830	13.1927
	$\widehat{\sigma}^2_{1,m_2}$	0.0122	0.0139	0.0197	0.0258	0.0390	0.0543	0.1997	0.7115	2.5678	14.8997
	$\widehat{\sigma}^2_{1,REML}$	0.0177	0.0227	0.0460	0.0592	0.0915	0.1108	0.4229	1.5222	4.5663	25.9121
	$\widehat{\sigma}^2_{1,ML}$	0.0050	0.0075	0.0156	0.0216	0.0400	0.0501	0.2177	0.8233	2.5913	14.8623
5	$\widehat{\sigma}^2_{1,u_1}$	0.0149	0.0156	0.0256	0.0484	0.0631	0.0957	0.4381	1.3197	4.4046	28.6096
	$\widehat{\sigma}^2_{1,u_2}$	0.0174	0.0191	0.0354	0.0578	0.0775	0.1228	0.5881	1.6704	5.4763	38.2848
	$\widehat{\sigma}^2_{1,m_1}$	0.0032	0.0033	0.0061	0.0129	0.0204	0.0302	0.1665	0.5750	2.1864	13.3664
	$\widehat{\sigma}^2_{1,m_2}$	0.0029	0.0033	0.0067	0.0131	0.0213	0.0331	0.1857	0.6303	2.4277	15.1549
	$\widehat{\sigma}^2_{1,REML}$	0.0118	0.0129	0.0189	0.0434	0.0578	0.0988	0.3894	1.2360	4.1832	27.1272
	$\widehat{\sigma}^2_{1,ML}$	0.0035	0.0042	0.0068	0.0175	0.0273	0.0454	0.2088	0.6882	2.4131	14.8074
6	$\widehat{\sigma}^2_{1,u_1}$	0.0248	0.0284	0.0377	0.0529	0.0721	0.0956	0.3129	0.9883	3.3501	20.3179
	$\widehat{\sigma}^2_{1,u_2}$	0.0272	0.0253	0.0380	0.0583	0.0758	0.1070	0.3227	1.0370	3.4599	21.6717
	$\widehat{\sigma}^2_{1,m_1}$	0.0061	0.0073	0.0101	0.0166	0.0245	0.0350	0.1407	0.4907	1.8164	10.7648
	$\widehat{\sigma}^2_{1,m_2}$	0.0087	0.0080	0.0122	0.0198	0.0276	0.0399	0.1482	0.5039	1.8648	11.0945
	$\widehat{\sigma}^2_{1,REML}$	0.0119	0.0117	0.0203	0.0392	0.0514	0.0735	0.2815	0.9111	3.1506	18.7353
	$\widehat{\sigma}^2_{1,ML}$	0.0048	0.0048	0.0090	0.0196	0.0288	0.0429	0.1781	0.5855	2.0512	11.9087

Table 5: Estimated Biases for estimators of σ_1^2, based on 10 different values of σ_1^2, $\mu = 0$, $\sigma_2^2 = 0.05$ and $\sigma_e^2 = 0.9$ with $N = 1000$ simulations

		σ_1^2									
Ex	est.	0.001	0.01	0.05	0.1	0.15	0.2	0.5	1.0	2.0	5.0
1	$\widehat{\sigma}^2_{1,u_1}$	0.0168	-0.0105	-0.0133	-0.0320	-0.0031	0.0369	-0.0012	-0.0141	-0.0702	-0.2245
	$\widehat{\sigma}^2_{1,m_1}$	0.0257	0.0112	-0.0164	-0.0553	-0.0796	-0.1004	-0.3125	-0.6499	-1.3351	-3.3860
	$\widehat{\sigma}^2_{1,REML}$	0.1290	0.1109	0.1021	0.0796	0.1013	0.1300	0.0814	0.0541	-0.115	-0.1802
	$\widehat{\sigma}^2_{1,ML}$	0.0438	0.0317	0.0043	-0.0328	-0.0505	-0.0630	-0.2467	-0.5142	-1.0530	-2.6414
2	$\widehat{\sigma}^2_{1,u_1}$	0.0047	-0.0208	0.0178	0.0050	0.0396	-0.0283	-0.0110	-0.0100	0.0078	0.3624
	$\widehat{\sigma}^2_{1,u_2}$	0.0056	-0.0220	0.0188	0.0051	0.0421	-0.0278	-0.0119	-0.0059	0.0029	0.3662
	$\widehat{\sigma}^2_{1,m_1}$	0.0233	0.0090	-0.0047	-0.0420	-0.0643	-0.1198	-0.3140	-0.6476	-1.3079	-3.1896
	$\widehat{\sigma}^2_{1,m_2}$	0.0237	0.0086	-0.0043	-0.0419	-0.0634	-0.1196	-0.3142	-0.6462	-1.3094	-3.1882
	$\widehat{\sigma}^2_{1,REML}$	0.1389	0.1087	0.1411	0.1243	0.1452	0.0820	0.0746	0.0650	0.0622	0.4129
	$\widehat{\sigma}^2_{1,ML}$	0.0493	0.0284	0.0194	-0.0156	-0.0325	-0.0901	-0.2573	-0.5117	-1.0236	-2.3457
3	$\widehat{\sigma}^2_{1,u_1}$	-0.0087	-0.0282	0.0441	-0.0342	-0.0017	0.0169	0.0288	0.0139	-0.0226	-0.0169
	$\widehat{\sigma}^2_{1,u_2}$	-0.0035	-0.0284	0.0390	-0.0355	-0.0011	0.0187	0.0308	0.0217	-0.0264	-0.0142
	$\widehat{\sigma}^2_{1,m_1}$	0.0254	0.0131	0.0095	-0.0498	-0.0718	-0.0988	-0.2950	-0.6332	-1.3112	-3.3106
	$\widehat{\sigma}^2_{1,m_2}$	0.0275	0.0136	0.0083	-0.0496	-0.0710	-0.0977	-0.2939	-0.6301	-1.3119	-3.3091
	$\widehat{\sigma}^2_{1,REML}$	0.1602	0.1453	0.1875	0.1180	0.1359	0.1597	0.1326	0.1177	0.0608	0.0448
	$\widehat{\sigma}^2_{1,ML}$	0.0468	0.0374	0.0313	-0.0301	-0.0569	-0.0705	-0.2496	-0.5153	-1.0501	-2.5660
4	$\widehat{\sigma}^2_{1,u_1}$	-0.0025	0.0035	-0.0071	-0.0068	-0.0093	0.0012	0.0012	0.0020	0.0003	0.0930
	$\widehat{\sigma}^2_{1,u_2}$	-0.0162	0.0068	-0.0015	-0.0054	-0.0320	-0.0036	0.0108	-0.0004	0.0318	0.1519
	$\widehat{\sigma}^2_{1,m_1}$	0.0098	0.0097	-0.0185	-0.0417	-0.0687	-0.0872	-0.2409	-0.4966	-1.0026	-2.4809
	$\widehat{\sigma}^2_{1,m_2}$	0.0047	0.0088	-0.0176	-0.0486	-0.0886	-0.1058	-0.2750	-0.5710	-1.1404	-2.8384
	$\widehat{\sigma}^2_{1,REML}$	0.0497	0.0539	0.0329	0.0287	0.0060	0.0214	0.0032	-0.0219	-0.0377	0.0552
	$\widehat{\sigma}^2_{1,ML}$	0.0218	0.0189	-0.0102	-0.0324	-0.0645	-0.0751	-0.1946	-0.3794	-0.7295	-1.6692
5	$\widehat{\sigma}^2_{1,u_1}$	-0.0007	-0.0047	-0.0017	-0.0058	0.0091	0.0165	-0.0237	-0.0215	-0.0087	-0.0984
	$\widehat{\sigma}^2_{1,u_2}$	-0.0021	-0.0068	-0.0011	-0.0023	0.0061	0.0139	-0.0447	-0.0123	0.0010	-0.1157
	$\widehat{\sigma}^2_{1,m_1}$	0.0045	-0.0016	-0.0212	-0.0499	-0.0691	-0.0912	-0.2680	-0.5301	-1.0496	-2.6685
	$\widehat{\sigma}^2_{1,m_2}$	0.0025	-0.0048	-0.0259	-0.0557	-0.0816	-0.1077	-0.3079	-0.5878	-1.1688	-2.9767
	$\widehat{\sigma}^2_{1,REML}$	0.0375	0.0319	0.0296	0.0187	0.0246	0.0351	-0.0174	-0.0175	0.0125	-0.1187
	$\widehat{\sigma}^2_{1,ML}$	0.0163	0.0075	-0.0121	-0.0367	-0.0511	-0.0615	-0.2017	-0.3667	-0.6881	-1.7696
6	$\widehat{\sigma}^2_{1,u_1}$	-0.0001	0.0020	-0.0049	0.0003	0.0137	-0.0071	0.0022	-0.0481	0.0465	0.0970
	$\widehat{\sigma}^2_{1,u_2}$	-0.0048	-0.0025	0.0005	-0.0044	0.0127	-0.0031	0.0165	-0.0466	0.0319	0.0711
	$\widehat{\sigma}^2_{1,m_1}$	0.0088	0.0065	-0.0130	-0.0326	-0.0440	-0.0775	-0.1970	-0.4318	-0.7952	-2.0115
	$\widehat{\sigma}^2_{1,m_2}$	0.0047	0.0021	-0.0137	-0.0381	-0.0501	-0.0808	-0.2000	-0.4530	-0.8428	-2.1236
	$\widehat{\sigma}^2_{1,REML}$	0.0422	0.0407	0.0257	0.0170	0.0311	0.0113	0.0004	-0.0430	0.0332	0.0614
	$\widehat{\sigma}^2_{1,ML}$	0.0223	0.0181	-0.0056	-0.0271	-0.0322	-0.0616	-0.1500	-0.3051	-0.4986	-1.226

Table 6: The observed Probability of obtaining negative estimates of σ_1^2 based on 10 different σ_1^2, $\mu = 0$, $\sigma_2^2 = 0.05$ and $\sigma_e^2 = 0.9$ with $N = 1000$ simulations

		σ_1^2									
Ex	est.	0.001	0.01	0.05	0.1	0.15	0.2	0.5	1.0	2.0	5.0
1	$\widehat{\sigma}^2_{1,u_1}$	0.6460	0.6430	0.5800	0.5690	0.5110	0.4890	0.4230	0.3240	0.2180	0.1690
	$\widehat{\sigma}^2_{1,m_1}$	0.5690	0.5670	0.5190	0.4870	0.4400	0.4280	0.3640	0.2690	0.1930	0.1510
2	$\widehat{\sigma}^2_{1,u_1}$	0.6460	0.6370	0.5820	0.5800	0.5240	0.4880	0.3920	0.3230	0.2510	0.1580
	$\widehat{\sigma}^2_{1,u_2}$	0.6350	0.6450	0.5900	0.5740	0.5310	0.4910	0.3960	0.3240	0.2470	0.1590
	$\widehat{\sigma}^2_{1,m_1}$	0.5690	0.5750	0.5120	0.5070	0.4660	0.4290	0.3430	0.2790	0.2070	0.1400
	$\widehat{\sigma}^2_{1,m_2}$	0.5690	0.5680	0.5170	0.5000	0.4600	0.4350	0.3460	0.2850	0.2070	0.1390
3	$\widehat{\sigma}^2_{1,u_1}$	0.6400	0.6190	0.6000	0.5920	0.5450	0.5220	0.4040	0.3610	0.2750	0.1880
	$\widehat{\sigma}^2_{1,u_2}$	0.6410	0.6260	0.6030	0.5860	0.5450	0.5300	0.3990	0.3530	0.2720	0.1950
	$\widehat{\sigma}^2_{1,m_1}$	0.5560	0.5420	0.5160	0.5230	0.4880	0.4610	0.3540	0.3040	0.2240	0.1610
	$\widehat{\sigma}^2_{1,m_2}$	0.5660	0.5490	0.5390	0.5150	0.4800	0.4580	0.3390	0.3090	0.2370	0.1660
4	$\widehat{\sigma}^2_{1,u_1}$	0.5390	0.5150	0.4330	0.3850	0.3650	0.3230	0.2020	0.1270	0.0640	0.0240
	$\widehat{\sigma}^2_{1,u_2}$	0.6020	0.5790	0.5450	0.4990	0.4760	0.4210	0.3000	0.2200	0.1300	0.0650
	$\widehat{\sigma}^2_{1,m_1}$	0.5410	0.5210	0.4220	0.3740	0.3440	0.2980	0.1860	0.1210	0.0590	0.0250
	$\widehat{\sigma}^2_{1,m_2}$	0.5640	0.5390	0.5010	0.4700	0.4470	0.3860	0.2790	0.2010	0.1200	0.0580
5	$\widehat{\sigma}^2_{1,u_1}$	0.6020	0.5860	0.4690	0.4300	0.3630	0.2660	0.1840	0.0990	0.0470	0.0160
	$\widehat{\sigma}^2_{1,u_2}$	0.6440	0.6090	0.5080	0.4500	0.3920	0.3200	0.2340	0.1400	0.062	00.0190
	$\widehat{\sigma}^2_{1,m_1}$	0.5700	0.5450	0.4460	0.3940	0.3400	0.2400	0.1730	0.0890	0.0380	0.0110
	$\widehat{\sigma}^2_{1,m_2}$	0.6180	0.5780	0.4770	0.4250	0.3700	0.3010	0.2150	0.1270	0.0560	0.0180
6	$\widehat{\sigma}^2_{1,u_1}$	0.5380	0.4970	0.4250	0.3760	0.3160	0.2330	0.1210	0.0660	0.0220	0.0060
	$\widehat{\sigma}^2_{1,u_2}$	0.6030	0.5690	0.4760	0.4070	0.3410	0.2880	0.1590	0.0800	0.0340	0.0090
	$\widehat{\sigma}^2_{1,m_1}$	0.5370	0.05020	0.3980	0.3370	0.2940	0.2120	0.1020	0.0520	0.0180	0.0050
	$\widehat{\sigma}^2_{1,m_2}$	0.5700	0.5370	0.4460	0.3700	0.3130	0.2610	0.1460	0.0730	0.0330	0.0070

Table 7: The observed MSE for estimation of σ_1^2 based on $\sigma_2^2/\sigma_1^2 = 0.8$, $\mu = 0$, $\sigma_2^2 = 0.05$ and $\sigma_e^2 = 0.9$ with $N = 1000$ simulations

		$\sigma_2^2/\sigma_1^2 = 0.8$					
Ex	est.	0.8,1	4,5	12,15	24,30	40,50	80,100
	$\widehat{\sigma}^2_{1,u_1}$	2.8979	57.3405	423.4799	995.3098	4847.170	19240.168
2	$\widehat{\sigma}^2_{1,u_2}$	2.9417	56.0465	420.1413	1015.9780	4848.737	19415.408
	$\widehat{\sigma}^2_{1,m_1}$	0.7336	17.3185	145.6219	383.3311	1657.436	6583.363
	$\widehat{\sigma}^2_{1,m_2}$	0.7399	17.2168	145.4236	384.9611	1653.197	6612.680
	$\widehat{\sigma}^2_{1,u_1}$	1.7133	34.8602	267.2678	1204.2242	3348.202	12375.354
5	$\widehat{\sigma}^2_{1,u_2}$	1.7311	36.6264	274.2066	1221.0254	3351.043	13188.749
	$\widehat{\sigma}^2_{1,m_1}$	0.6093	13.5307	113.3753	475.6935	1356.286	5197.689
	$\widehat{\sigma}^2_{1,m_2}$	0.6408	14.9743	125.7473	520.3050	1447.766	5734.068

3.5 Case 5: The effect of the number of observations on the MSE

The difference in MSE between the variance component estimators decreased for large n (Figure 1). The MSEs of $\widehat{\sigma}^2_{1,u_1}$ were more sensitive for the changes in n than $\widehat{\sigma}^2_{1,m_1}$ and $\widehat{\sigma}^2_{1,ML}$. If n was large enough, then the MSEs of the estimators were approximately equal and the unbiased estimators should be preferred.

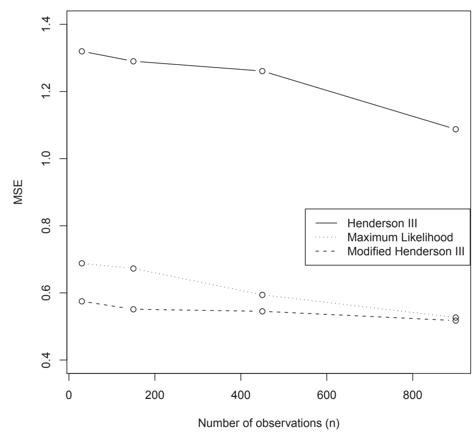

Figure 1: Observed MSE for different n=30,150,450,900. The simulated variance components were $\sigma_2^2 = 0.05$,$\sigma_1^2 = 1$, $\sigma_e^2 = 0.09$. MSE calculated from 1000 simulation replicates. Partition I was used for the Henderson III and modified Henderson III estimates.

4 Conclusion

The main conclusion from our simulation study is that in terms of MSE and probability of obtaining negative estimators, the modified estimators from the two partitions perform better than their non-modified corresponding estimators. However, when unbiasedness is the main concern, the (non-modified) Henderson's 3 estimators and the REML estimator are preferred. The simulation results also give a guideline for when to choose partition I rather than partition II. Further, the results show that when n is large and the MSE is the main concern, $\widehat{\sigma}^2_{1,m_1}$ can be preferred over the other considered estimators i.e., $\widehat{\sigma}^2_{1,u_1}$, $\widehat{\sigma}^2_{1,u_2}$ and $\widehat{\sigma}^2_{1,m_2}$.

Regarding imbalance, $\widehat{\sigma}^2_{1,m_1}$ is more robust and performs better than $\widehat{\sigma}^2_{1,u_1}$. Furthermore, if MSE is of interest, the $\widehat{\sigma}^2_{1,ML}$ and $\widehat{\sigma}^2_{1,m_1}$ are very close and have lower MSE than all the other considered estimators. Moreover, for all the considered examples the modified variance component estimators have in general a lower MSE than their corresponding non-modified ones. Further, the probability of obtaining negative estimates was smaller for the modified variance component estimators than the non-modified ones.

Hence, our simulation study gives improved insight to the biasedness and accuracy of modified Henderson's method 3 for variance component estimation. Besides giving insight to variance component estimators in general, our results give guidelines for applied research (e.g. Rönnegård et al. 2009).

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Appendix

A Expressions for the reduction sum of squares needed for Henderson's method 3

To estimate the variance components of the model (2.1) we define the following matrices $[X]$, $[X, Z_1]$ and $[X, Z_1, Z_2]$. The corresponding projection matrices are

$$\begin{aligned} P_x &= X(X'X)^{-}X', \\ P_{x_1} &= (X, Z_1)((X, Z_1)'(X, Z_1))^{-}(X, Z_1)', \\ P_{x_{12}} &= (X, Z_1, Z_2)((X, Z_1, Z_2)'(X, Z_1, Z_2))^{-}(X, Z_1, Z_2)', \end{aligned}$$

where $^{-}$ represents the g-inverse $AA^{-}A = A$. The first set of estimation equation partition I is based on

$$\begin{cases} \mathrm{R}(u_1/\beta) \\ \mathrm{R}(u_2/\beta, u_1) \\ \mathrm{SSE} \end{cases}$$

where $\mathrm{R}(\cdot)$ denotes the reduction sum of squares, $\mathrm{R}(u_1/\beta) = Y'(P_{x_1} - P_x)Y$, $\mathrm{R}(u_2/\beta, u_1) = Y'(P_{x_{12}} - P_{x_1})Y$ and the residual sum of squares is denoted by $\mathrm{SSE} = Y'(I - P_{x_{12}})Y$, see Searle (1971). The obtained variance component estimator from partition I is

$$\begin{aligned} \widehat{\sigma}^2_{1,u_1} &= \frac{Y'(P_{x_1} - P_x)Y}{tr(P_{x_1} - P_x)V_1} - \frac{tr(P_{x_1} - P_x)V_2 Y'(P_{x_{12}} - P_{x_1})Y}{tr(P_{x_1} - P_x)V_1 tr(P_{x_{12}} - P_{x_1})V_2} \\ &\quad + \frac{kY'(I - P_{x_{12}})Y}{tr(P_{x_1} - P_x)V_1 tr(P_{x_{12}} - P_{x_1})V_2 tr(I - P_{x_{12}})}. \end{aligned} \tag{A.1}$$

The modified variance component estimator given by Al-Sarraj and von Rosen (2009) is as below:

$$\begin{aligned} \widehat{\sigma}^2_{1,m_1} &= c_1\Big(\frac{Y'(P_{x_1} - P_x)Y}{tr(P_{x_1} - P_x)V_1} - \frac{tr(P_{x_1} - P_x)V_2 d_1 Y'(P_{x_{12}} - P_{x_1})Y}{tr(P_{x_1} - P_x)V_1 tr(P_{x_{12}} - P_{x_1})V_2} \\ &\quad + \frac{kd_2 Y'(I - P_{x_{12}})Y}{tr(P_{x_1} - P_x)V_1 tr(P_{x_{12}} - P_{x_1})V_2 tr(I - P_{x_{12}})}\Big). \end{aligned} \tag{A.2}$$

For the coefficients c_1, d_1 and d_2 given in (A.2) we have the following values

$$\begin{aligned}
c_1 &= \frac{1}{\frac{2}{[tr(P_{x_1}-P_x)V_1]^2}[tr(P_{x_1}-P_x)V_1(P_{x_1}-P_x)V_1]+1}, \\
d_1 &= \frac{1}{\frac{2}{[tr(P_{x_{12}}-P_{x_1})V_2]^2}[tr(P_{x_{12}}-P_{x_1})V_2(P_{x_{12}}-P_{x_1})V_2]+1}, \\
d_2 &= \frac{\frac{(tr(P_{x_1}-P_x)V_2)}{tr(P_{x_{12}}-P_{x_1})V_2}d_1 tr(P_{x_{12}}-P_{x_1})-tr(P_{x_1}-P_x)}{[\frac{k}{tr(P_{x_{12}}-P_{x_1})V_2}][\frac{2}{tr(I-P_{x_{12}})}+1]},
\end{aligned}$$

where $V_1 = Z_1Z_1'$, $V_2 = Z_2Z_2'$ and $k = tr((P_{x_1} - P_x)V_2)tr(P_{x_{12}} - P_{x_1}) - tr(P_{x_1} - P_x)tr((P_{x_{12}} - P_{x_1})V_2)$. For details and calculations see Al-Sarraj and von Rosen (2009). For the second set of estimation equations partition II we need to define $[X, Z_2]$ and the corresponding projection matrix

$$P_{x_2} = (X, Z_2)((X, Z_2)'(X, Z_2))^-(X, Z_2)'.$$

Partition II is based on the following set of equations

$$\begin{cases} \mathrm{R}(u_1/\beta, u_2) \\ \mathrm{SSE} \end{cases}$$

where $\mathrm{R}(u_1/\beta, u_2) = Y'(P_{x_{12}} - P_{x_2})Y$ and $\mathrm{SSE} = Y'(I - P_{x_{12}})Y$. The obtained variance component estimator from partition II is

$$\begin{aligned}
\widehat{\sigma}^2_{1,u_2} &= \frac{tr(I-P_{x_{12}})Y'(P_{x_{12}}-P_{x_2})Y - tr(P_{x_{12}}-P_{x_2})Y'(I-P_{x_{12}})Y}{tr(P_{x_{12}}-P_{x_2})V_2 tr(I-P_{x_{12}})} \\
&= \frac{Y'(P_{x_{12}}-P_{x_2})Y}{tr(P_{x_{12}}-P_{x_2})V_1} - \frac{tr(P_{x_{12}}-P_{x_2})Y'(I-P_{x_{12}})Y}{tr(P_{x_{12}}-P_{x_2})V_1 tr(I-P_{x_{12}})}. \qquad \text{(A.3)}
\end{aligned}$$

The modified variance component estimator of partition II is:

$$\widehat{\sigma}^2_{1,m_2} = \frac{c_2 Y'(P_{x_{12}}-P_{x_2})Y}{tr(P_{x_{12}}-P_{x_2})V_1} - \frac{c_2\varepsilon_1 tr(P_{x_{12}}-P_{x_2})Y'(I-P_{x_{12}})Y}{tr(P_{x_{12}}-P_{x_2})V_1 tr(I-P_{x_{12}})}. \qquad \text{(A.4)}$$

Now for the coefficients that are involved in partition II, i.e., c_2 and ε_1 given in (A.4) we refer to Kelly and Mathew (1994). However, we have calculated the values such that they would be appropriate for the second set of estimation equations partition II,

$$\begin{aligned}
c_2 &= \frac{1}{\frac{2}{[tr(P_{x_{12}}-P_{x_2})V_1]^2}[tr(P_{x_{12}}-P_{x_2})V_1(P_{x_{12}}-P_{x_2})V_1]+1}, \\
\varepsilon_1 &= \frac{1}{\frac{2}{tr(I-P_{x_{12}})}+1}.
\end{aligned}$$

B

For simplicity and before we write the mean square error equations for the variance component estimators obtained in (A.1), (A.2), (A.3) and (A.4) we define the following

$$A = (P_{x_1} - P_x), \quad B = (P_{x_{12}} - P_{x_1}), \quad C = (I - P_{x12}),$$
$$a = tr(P_{x_1} - P_x)V_1, \quad b = tr(P_{x12} - P_{x_1})V_2, \quad c = tr(I - P_{x_{12}}),$$
$$d = tr(P_{x_1} - P_x)V_2, \quad e = tr(P_{x_{12}} - P_{x_1}), \quad f = tr(P_{x_1} - P_x).$$

The MSEs for the non-modified and modified variance component estimators, i.e., $\widehat{\sigma}^2_{1,u_1}$ and $\widehat{\sigma}^2_{1,m_1}$ respectively, obtained from partition I are as follows:

(i) **The MSE of $\widehat{\sigma}^2_{1,u_1}$**

$$\begin{aligned} &\text{MSE}(\widehat{\sigma}^2_{1,u_1}) \\ = \; & [\frac{2}{a^2} tr(AV_1AV_1)]\sigma_1^4 + [\frac{2}{a^2} tr(AV_2AV_2) + \frac{2d^2}{a^2b^2} tr(BV_2BV_2)]\sigma_2^4 \\ & + [\frac{4}{a^2} tr(AV_1AV_2)]\sigma_1^2\sigma_2^2 + [\frac{4}{a^2} tr(AV_1A)]\sigma_1^2\sigma_e^2 \\ & + [\frac{4}{a^2} tr(AV_2A) + \frac{4d^2}{a^2b^2} tr(BV_2B)]\sigma_2^2\sigma_e^2 \\ & + [\frac{2}{a^2} tr(A^2) + \frac{2d^2}{a^2b^2} tr(B^2) + \frac{2k^2}{a^2b^2c^2} tr(C^2)]\sigma_e^4. \end{aligned} \tag{B.1}$$

(ii) **The MSE of $\widehat{\sigma}^2_{1,m_1}$**

$$\begin{aligned} &\text{MSE}(\widehat{\sigma}^2_{1,m_1}) \\ = \; & [\frac{2c_1^2}{a^2} tr(AV_1AV_1) + (c_1-1)^2]\sigma_1^4 + [\frac{4c_1^2}{a^2} tr(AV_1AV_2) + 2(c_1-1)r]\sigma_1^2\sigma_2^2 \\ & + [\frac{2c_1^2}{a^2} tr(AV_2AV_2) + \frac{2d^2c_1^2d_1^2}{a^2b^2} tr(BV_2BV_2) + r^2]\sigma_2^4 \\ & + [\frac{4c_1^2}{a^2} tr(A^2V_1) + 2(c_1-1)t]\sigma_1^2\sigma_e^2 \\ & + [\frac{4c_1^2}{a^2} tr(A^2V_2) + \frac{4d^2c_1^2d_1^2}{a^2b^2} tr(B^2V_2) + 2rt]\sigma_2^2\sigma_e^2 \\ & + [\frac{2c_1^2}{a^2} tr(A^2) + \frac{2d^2c_1^2d_1^2}{a^2b^2} tr(B^2) + \frac{2k^2c_1^2d_2^2}{a^2b^2c^2} tr(C^2) + t^2]\sigma_e^4, \end{aligned} \tag{B.2}$$

where

$$r = \frac{c_1 d}{a} - \frac{dc_1d_1}{a}, \quad t = \frac{c_1}{a} tr(A) - \frac{dc_1d_1}{ab} tr(B) + \frac{c_1kd_2}{ab}.$$

The following two equations give the MSEs for the variance component estimators obtained from partition II, i.e., $\widehat{\sigma}^2_{1,u_2}$ and $\widehat{\sigma}^2_{1,m_2}$:

(iii) **The MSE of $\widehat{\sigma}^2_{1,u_2}$**

$$\begin{aligned} &\mathrm{MSE}(\widehat{\sigma}^2_{1,u_2}) \\ &= [\tfrac{2tr(EV_1EV_1)}{g^2}]\sigma_1^4 + [\tfrac{4tr(EV_1E)}{g^2}]\sigma_1^2\sigma_e^2 + [\tfrac{2tr(E^2)}{g^2} + \tfrac{2l^2}{g^2c}]\sigma_e^4 \end{aligned} \quad \text{(B.3)}$$

where $E = P_{x_{12}} - P_{x_2}$, $g = tr((P_{x_{12}} - P_{x_2})V_1)$ and $l = tr(P_{x_{12}} - P_{x_2})$

(iv) **The MSE of $\widehat{\sigma}^2_{1,m_2}$**

$$\begin{aligned} &\mathrm{MSE}(\widehat{\sigma}^2_{1,m_2}) \\ =\ &[\frac{2c_2^2tr(EV_1EV_1)}{g^2} + (c_2-1)^2]\sigma_1^4 \\ &+ [\frac{4c_2^2tr(EV_1E)}{g^2} + 2(c_2-1)\frac{c_2l}{g}(1-\frac{l}{g})]\sigma_1^2\sigma_e^2 \\ &+ [\frac{2c_2^2tr(E^2)}{g^2} + \frac{2c_2^2\varepsilon_1^2l^2}{g^2c} + (\frac{c_2l}{g}(1-\frac{l}{g}))^2]\sigma_e^4 \end{aligned} \quad \text{(B.4)}$$

C

Example	The Model	n	p	q
1	$Y = 1_8\mu + \begin{pmatrix} 1_4 & 0 \\ 0 & 1_4 \end{pmatrix} u_1 + \begin{pmatrix} 1_2 & 0 \\ 0 & 1_2 \\ 1_2 & 0 \\ 0 & 1_2 \end{pmatrix} u_2 + e.$	8	2	2
2	$Y = 1_8\mu + \begin{pmatrix} 1_5 & 0 \\ 0 & 1_3 \end{pmatrix} u_1 + \begin{pmatrix} 1_2 & 0 \\ 0 & 1_3 \\ 1_1 & 0 \\ 0 & 1_2 \end{pmatrix} u_2 + e.$	8	2	2
3	$Y = 1_8\mu + \begin{pmatrix} 1_6 & 0 \\ 0 & 1_2 \end{pmatrix} u_1 + \begin{pmatrix} 1_4 & 0 \\ 0 & 1_2 \\ 1_1 & 0 \\ 0 & 1_1 \end{pmatrix} u_2 + e.$	8	2	2
4	$Y = 1_{21}\mu + \begin{pmatrix} 1_5 & 0 & 0 \\ 0 & 1_9 & 0 \\ 0 & 0 & 1_7 \end{pmatrix} u_1 + \begin{pmatrix} 1_2 & 0 & 0 \\ 0 & 1_3 & 0 \\ 0 & 1_1 & 0 \\ 0 & 0 & 1_8 \\ 1_4 & 0 & 0 \\ 0 & 1_3 & 0 \end{pmatrix} u_2 + e$	21	3	3
5	$Y = 1_{30}\mu + \begin{pmatrix} 1_{10} & 0 & 0 \\ 0 & 1_{15} & 0 \\ 0 & 0 & 1_5 \end{pmatrix} u_1 + \begin{pmatrix} 1_5 & 0 & 0 \\ 0 & 1_5 & 0 \\ 1_{10} & 0 & 0 \\ 0 & 1_5 & 0 \\ 0 & 1_2 & 0 \\ 0 & 0 & 1_3 \end{pmatrix} u_2 + e.$	30	3	3
6	$Y = 1_{30}\mu + \begin{pmatrix} 1_7 & 0 & 0 & 0 \\ 0 & 1_{12} & 0 & 0 \\ 0 & 0 & 1_6 & 0 \\ 0 & 0 & 0 & 1_5 \end{pmatrix} u_1 + \begin{pmatrix} 1_4 & 0 & 0 \\ 0 & 0 & 1_3 \\ 0 & 1_{10} & 0 \\ 0 & 0 & 1_2 \\ 1_2 & 0 & 0 \\ 0 & 1_4 & 0 \\ 1_5 & 0 & 0 \end{pmatrix} u_2 + e.$	30	4	3

D

The mean square error MSE of an estimator $\hat{\theta}$, denoted by MSE($\hat{\theta}$), can be defined as

$$MSE(\hat{\theta}) = D(\hat{\theta}) + (Bias(\hat{\theta}))^2,$$

where $D(\cdot)$ denotes the variance. The bias of an estimator $\widehat{\theta}$ of a parameter θ is the difference between the expected value of $\hat{\theta}$ and θ, i.e., $Bias(\hat{\theta}) = \mathrm{E}(\hat{\theta}) - \theta$.

Let $\hat{\sigma}^2$ be the estimator of the true value σ^2, the expectation and variance of $\hat{\sigma}^2$ denoted as $\mathrm{E}(\hat{\sigma}^2)$ and $\mathrm{D}(\hat{\sigma}^2)$, respectively and a sample set of data defined as $\hat{\sigma}^2 = (\hat{\sigma}_1^2, \hat{\sigma}_2^2, \cdots, \hat{\sigma}_N^2)$. Consequently, the observed sample mean of $\hat{\sigma}^2$ is:

$$mean(\hat{\sigma}^2) = \frac{1}{N}\sum \hat{\sigma}_i^2.$$

Here, mean($\hat{\sigma}^2$) replaces $\mathrm{E}(\hat{\sigma}^2)$. The observed sample variance denoted as $S^2(\hat{\sigma}^2)$ is obtained:

$$S^2(\hat{\sigma}^2) = \frac{1}{N-1}\sum(\hat{\sigma}_i^2 - mean(\hat{\sigma}^2))^2,$$

and here $S^2(\hat{\sigma}^2)$ replaces $\mathrm{D}(\hat{\sigma}^2)$. Thus, the estimated bias of $\hat{\sigma}^2$ is

$$Bias(\hat{\sigma}^2) = mean(\hat{\sigma}^2) - \sigma^2.$$

According to the definition, the mean square error of $\widehat{\sigma}^2$ is

$$MSE(\hat{\sigma}^2) = S^2(\hat{\sigma}^2) + [Bias(\hat{\sigma}^2)]^2.$$

The observed negative probability used in this study is

$$P(\hat{\sigma}^2 < 0) = Q/N,$$

where Q is the number of negative estimates.