

Comparison of REML and MINQUE for Estimated Variance Components and Predicted Random Effects

Nan Nan¹, Johnie N. Jenkins², Jack C. McCarty², Jixiang Wu^{3*}

¹Department of Mathematics and Statistics; South Dakota State University, Brookings, SD, USA ²Crop Science Research Laboratory USDA-ARS, Mississippi State, MS, USA ³Agronomy, Horticulture, and Plant Science Department, South Dakota State University, Brookings, SD, USA Email: *jixiang.wu@sdstate.edu

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Abstract

Linear mixed model (LMM) approaches have been widely applied in many areas of research data analysis because they offer great flexibility for different data structures and linear model systems. In this study, emphasis is placed on comparing the properties of two LMM approaches: restricted maximum likelihood (REML) and minimum norm quadratic unbiased estimation (MINQUE) with and without resampling techniques being included. Bias, testing power, Type I error, and computing time were compared between REML and MINQUE approaches with and without Jackknife technique based on 500 simulated data sets. Results showed that MINQUE and REML methods performed equally regarding bias, Type I error, and power. Jackknifebased MINQUE and REML greatly improved power compared to non-Jackknife based linear mixed model approaches. Results also showed that MINQUE is more timesaving compared to REML, especially with the use of resampling techniques and large data set analysis. Results from the actual cotton data analysis were in agreement with our simulated results. Therefore, Jackknife-based MINQUE approaches could be recommended to achieve desirable power with reduced time for a large data analysis and model simulations.

Keywords

Linear Mixed Model Approaches, MINQUE, REML, Jackknife

1. Introduction

Linear mixed models (LMM) are a generalization of various linear models covering simple linear regression models, ANOVA models, and complex genetic models. LMM approaches including maximum likelihood (ML) [1], restricted maximum likelihood (REML) [2], and minimum norm quadratic unbiased estimation (MINQUE) [3] are among the most commonly used ones for variance component estimation and random effect prediction. Numerical comparisons of the statistical properties among these LMM approaches could help users choose appropriate approaches for various data analyses.

ML and REML approaches have been integrated into SAS [4] and into R such as lme4 [5] [6] and ASReml [7]. Due to their popularity and long-term availability, a wide range of applications in various areas, has occurred. For example, based on a recent google scholar search in May, 2016, more than 43,000 publications were available. Both ML and REML approaches are based on the assumption that data are normally distributed (Laird and Ware, 1982) and require iterations [8]. Compared to ML and REML, MINQUE approaches were less popular. However, MINQUE approaches do not require normally distributed data nor iterations [3] [9]. Thus, they could offer more flexibility with reduced computational intensity. Since 1989, MINQUE approaches have been widely used in quantitative genetics studies [10]-[19].

Though LMM approaches are currently widely used, a potential issue associated with LMM is low power in statistical tests for variance components and random effects. With the use of jackknife methods, statistical powers could be significantly improved [20]-[22]. On the other hand, with resampling techniques, it is possible to generalize statistical tests for various parameters of interest. Resampling techniques including jackknife and permutation methods have been integrated in linear mixed model approaches and two R packages, minque and qgtools, which are currently available online [23] [24].

The aim of this study was to compare statistical properties between REML and MINQUE approaches with and without a jackknife technique [25] through Monte Carlo simulations. A cotton data set [25] including 24 genotypes under two environments was used for both simulations and actual data analyses. These methods were compared regarding statistical power, Type I error, and computational time. Results including variance components and genotypic effects from actual data analysis were also compared. Results could provide statistical information on appropriate use of these LMM approaches.

2. Materials and Methods

2.1. Materials

Various data structures and related linear mixed models can be used for our simulations and actual data analysis. Without losing our focus of this study, we employed a cotton data set including 24 cotton genotypes under two locations each following a randomized complete block design with six replications [25]. The data were collected on the two sites at the research farm at Mississippi State University, Starkville, MS. The data structure was used for simulation study using the model detailed below (Equation (1)). Two agronomic traits: lint yield (LY), and lint percentage (LP), were included and used for our actual data analysis. The data set, cot, is currently available in the R package, minque [23].

2.2. Statistical Model and Methods

Given the data structure, the observation y_{ijk} standing for the genotype *j* under the k^{th} block in the environment *i* can be expressed by using the following linear mixed model:

$$y_{ijk} = \mu + E_i + G_j + GE_{ij} + B_{k(i)} + e_{ijk}$$
(1)

where E_i is an environmental effect and treated as fixed effect; G_j is a genotypic effect and treated as random; GE_{ij} is a genotype-by-environment interaction effect and random; $B_{k(i)}$ is a random block effect within environment; and e_{ijk} is the random error.

Two linear mixed model approaches, MINQUE and REML [2] [3] [9], were applied. In addition, a randomized 10-fold Jackknife technique [21] was integrated with these two linear mixed model approaches. Therefore, four combinations of methods in total were used for both simulation and actual data analysis. To simplify our description, we defined these four combinations of methods as: M1 = MINQUE without jackknife; M2 = REML without jackknife; M3 = MINQUE with jackknife; and M4 = REML with jackknife. Regarding simulation studies, there could be numerous parameter settings, however, we only considered two representative parameter settings because the major aim of this study was to compare statistical properties among these four methods. The first setting was to preset all variance components to 20 (interested users may use other settings), targeting power and bias. The second setting was to preset all variance components to zero except the random error variance which was 20, targeting Type I error and bias for all variance components except random error variance. For each parameter setting, five hundred simulated data sets [26] [27] were generated and analyzed by each combination of these four methods. Statistical properties including bias, and testing power/Type I error were calculated for each method [28] [29]. Type I error is the false significance rate for a preset variance component being zero while testing power is the true significance rate for a positive preset variance component over 500 simulations. The bias is for each variance component is the deviation of mean estimated variance component from the preset variance component (0 or 20 in this study) which is given by Equation (2):

$$Bias = \overline{\hat{\theta}} - \theta_0 \tag{2}$$

where, θ_0 is a preset variance component and $\overline{\hat{\theta}}$ is mean estimated variance component. We briefly defined the following terms. The standard error (*SE*) is defined by $SE(\overline{\hat{\theta}})$, a standard error for a mean estimated variance component. In addition, computational time (in seconds) was recorded for every 100 simulations out of 500 simulations (**Table 3**).

For actual data analysis, variance components were estimated by REML and MINQUE approaches and genotypic effects were predicted by the adjusted unbiased prediction method [30]. All simulations and data analyses were conducted using the

functions that are available in the R package minque [23] under the R Studio environment [31]. The computational time recorded for simulation was based on HP Z440 with 32G ram under Windows 7 64-bit operation system.

3. Results and Discussion

3.1. Simulation Results

Bias, standard error, power, Type I error, and computational time based on 500 simulated data for four methods are summarized in Table 1 and Table 2. Results showed that bias for each variance component was similar among the four methods (M1-M4) (Table 1 and Table 2). Standard errors (SE) for each variance component among 500 estimates were also similar for the four methods (Table 1 and Table 2). Non-Jackknife based MINQUE and REML methods (M1 and M2) had similar power (at the probability level of 5%). However, Jackknife based REML and MINQUE methods (M3 and M4) had improved power for variances of genotypic and block effects compared to non-Jackknife based methods(M1 and M2) (Table 1). All four methods yield acceptable Type I error (around 5% or lower) for all variance components except the random error variance component (Table 2). Overall, both MINQUE and REML performed equally well regarding bias, power, and Type I error for variance component estimation. However, jackknife based MINQUE and REML could greatly improve power with acceptable Type I error compared to non-jackknife based methods.

Computational time in seconds used for each 100 simulations for each method and parameter setting is given in Table 3. Though other tasks were possible active during

Table 1. Estimated bias, standard error (SE), and power (at 0.05) for four preset components based on 500 simulated data sets with four methods.

			$M1^{\rm H}$			M2	
	Parameter	Bias	SE	Power	Bias	SE	Power
$V_{_G}$ *	20	0.041	0.461	0.664	0.033	0.461	0.666
$V_{\scriptscriptstyle GE}$	20	0.022	0.319	1.000	0.013	0.318	1.000
$V_{\scriptscriptstyle B}$	20	-0.263	0.505	0.786	-0.263	0.505	0.788
$V_{_e}$	20	0.024	0.080	1.000	0.026	0.080	1.000
			M3			M4	
	Parameter	Bias	SE	Power	Bias	SE	Power
$V_{_G}$	20	0.044	0.461	0.944	0.044	0.462	0.934
$V_{\scriptscriptstyle GE}$	20	0.016	0.319	1.000	0.007	0.318	1.000
$V_{_B}$	20	-0.260	0.505	0.998	-0.263	0.505	0.998
$V_{_e}$	20	0.025	0.080	1.000	0.027	0.080	1.000

ⁱ: M1 = MINQUE approach without Jackknife; M2 = REML approach without Jackknife; M3 = MINQUE approach with Jackknife; and M4 = REML approach with Jackknife

[†]: V_G = variance component for genotype effects; V_{GE} = variance component for genotype and environment interaction effects; V_B = variance component for block effects; and V_e = variance component for random error.

			$M1^{\rm H}$			M2	
	Parameter	Bias	SE	Type I error	Bias	SE	Type I error
$V_{_G}{}^{\dagger}$	0	0.041	0.461	0.012	0.033	0.461	0.002
$V_{\scriptscriptstyle GE}$	0	0.022	0.319	0.006	0.013	0.318	0.000
$V_{\scriptscriptstyle B}$	0	-0.263	0.505	0.000	-0.263	0.505	0.000
$V_{_e}$	20	0.024	0.080	1.000	0.026	0.080	1.000
			M3			M4	
	Parameter	Bias	SE	Type I error	Bias	SE	Type I error
$V_{_G}$	0	0.044	0.461	0.058	0.044	0.462	0.048
$V_{_{GE}}$	0	0.016	0.319	0.034	0.007	0.318	0.040
$V_{\scriptscriptstyle B}$	0	-0.260	0.505	0.024	-0.263	0.505	0.042
$V_{_e}$	20	0.025	0.080	1.000	0.027	0.080	1.000

Table 2. Estimated bias, standard error (SE), and Type I error (at 0.05) for four preset components based on 500 simulated data sets with four methods.

¹: M1 = MINQUE approach without Jackknife; M2 = REML approach without Jackknife; M3 = MINQUE approach with Jackknife; and M4 = REML approach with Jackknife

[†]: V_G =variance component for genotype effects; V_{GL} = variance component for genotype and environment interaction effects; V_B = variance component for block effects; and V_e = variance component for random error.

		Parame	ter setting 1 ^H			Parameter setting 2			
	$M1^{\dagger}$	M2	M3	M4	M1	M2	M3	M4	
1 st 100	14.8	17.6	18.4	157.8	10.7	20.7	10.6	189.6	
2nd 100	13.0	15.9	18.1	153.6	10.8	20.6	10.7	188.4	
3 rd 100	13.1	16.0	18.1	154.2	10.7	19.5	10.3	184.2	
$4^{th} \ 100$	13.1	16.1	17.9	154.8	10.9	20.6	10.8	193.8	
5 th 100	12.9	15.9	18.5	154.2	10.8	21.2	11.6	198.6	
Total	66.9	81.5	91.0	774.6	53.9	102.6	54.0	954.6	

Table 3. Computational time (seconds) recorded each 100 simulations out of 500 simulations for each method and parameter setting.

ⁱ: Parameter settings 1: all variance components were preset as 20; Parameter settings 2: all variance components were preset as 0 except the error variance component being set to 20.

: M1 = MINQUE approach without Jackknife; M2 = REML approach without Jackknife; M3 = MINQUE approach with Jackknife; and M4 = REML approach with Jackknife.

the simulation process, computational time among five 100-simulations was similar given a particular parameter setting and method. Among four methods, M1, M2, and M3 were time-saving (less than two minutes) while M4 took much longer (over 10 minutes) than the other three methods. For parameter setting 1, M2 (REML without jackknife) took 14.6 seconds longer than M1 (MINQUE without jackknife) and M3 (MINQUE with jackknife) was only 24.1 seconds longer than M1 over 500 simulations (**Table 3**). For parameter setting 2, M2 (REML without jackknife) was little longer than M1 and M3, which had similar computing time. M1 and M3 appeared more time-saving

for the parameter setting 2 compared to the parameter setting 1. Our repeated simulations showed the same pattern (results not shown). One possible reason is that REML may need more iterations to converge for zero or negative variance components than for positive variance components. M4 was over eight-fold slower compared to M3 for the parameter setting 1 while 17 times slower for the parameter setting 2. Therefore, the results showed that MINQUE approach with or with jackknife was very time-saving yet yielded almost identical results compared to REML approach especially integrated with resampling process.

3.2. Actual Data Analysis

With the same model, two agronomic traits: cotton lint yield (LY) and lint percentage (LP), were analyzed by the same four methods used in our simulation studies. Estimated variance components for these two traits are summarized in Table 4 and Table 5 while predicted genotypic effects are presented in Table 6 and Table 7. Results showed that estimated variance components were similar for four methods for each of two traits while M3 and M4 yielded smaller standard error compared to M1 and M2 (Table 4 and Table 5). On the other hand, all four methods yielded similar predicted genotypic effects while M3 and M4 had lower standard errors compared to M1 and M2 (Table 6 and Table 7). The results in Tables 4-7 showed that Jackknife technique integrated

Table 4. Estimated variance components for lint yield (LY) by four methods.

Daramatar	$M1^{H}$		M2		M3		M4	
Falameter	Est	SE	Est	SE	Est	SE	Est	SE
$V_{_G}$	52,068	16,220	50,356	16,031	52,395	1567	50,548	1137
$V_{\scriptscriptstyle GL}$	333	1230	2379	2105	502	538	2322	681
$V_{\scriptscriptstyle B}$	838	890	848	890	803	324	806	335
$V_{_e}$	25,168	2296	24,799	2275	25,312	888	24,904	833

^I: M1 = MINQUE approach without Jackknife; M2 = REML approach without Jackknife; M3 = MINQUE approach with Jackknife; and M4 = REML approach with Jackknife

[†]: V_G = variance component for genotype effects; V_{GL} = variance component for genotype and location interaction effects; V_B = variance component for block effects; and V_e = variance component random error.

Table 5. Estimated variance components for lint percentage (LP) by four methods.

Parameter	M1 ^I		M2		M3		M4	
	Est	SE	Est	SE	Est	SE	Est	SE
$V_{_G}$	9.661	2.977	9.299	2.877	9.720	0.247	9.296	0.252
$V_{\scriptscriptstyle GL}$	0.460	0.242	0.509	0.260	0.513	0.276	0.537	0.176
$V_{\scriptscriptstyle B}$	0.129	0.103	0.128	0.103	0.132	0.036	0.128	0.016
$V_{_e}$	1.798	0.166	1.805	0.166	1.774	0.159	1.790	0.085

ⁱ: M1 = MINQUE approach without Jackknife; M2 = REML approach without Jackknife; M3 = MINQUE approach with Jackknife; and M4 = REML approach with Jackknife

ⁱ: V_G = variance component for genotype effects; V_{GL} = variance component for genotype and location interaction effects; V_B = variance component for block effects; and V_e = variance component random error.

	M1 [±]		M2	M2		M3		M4	
Genotype	Pre	SE	Pre	SE	Pre	SE	Pre	SE	
1	-249.93	217	-247.035	211	-250.06	15.07	-246.80	11.76	
2	-269.19	217	-266.164	211	-268.78	26.76	-264.52	12.60	
3	-28.47	217	-27.174	211	-28.77	15.36	-27.45	13.86	
4	-366.26	217	-362.525	211	-365.41	11.11	-360.95	12.13	
5	-251.01	217	-248.111	211	-250.99	9.19	-247.62	13.16	
6	-34.13	217	-32.793	211	-33.67	23.36	-32.02	22.83	
7	84.73	217	85.208	211	83.92	10.31	83.97	12.85	
8	3.56	217	4.628	211	2.44	11.19	4.30	9.09	
9	-11.85	217	-10.675	211	-12.21	24.11	-8.97	23.65	
10	-126.61	217	-124.611	211	-126.88	21.16	-126.25	16.76	
11	-24.49	217	-23.229	211	-25.97	21.13	-23.45	10.85	
12	97.13	217	97.522	211	95.42	33.32	96.34	30.43	
13	-2.94	217	-1.828	211	-3.80	11.92	-2.50	17.69	
14	-180.68	217	-178.291	211	-179.72	16.40	-177.87	15.22	
15	-164.55	217	-162.271	211	-163.10	21.15	-162.73	30.91	
16	95.21	217	95.609	211	94.91	10.76	94.96	12.99	
17	-215.73	217	-213.082	211	-215.76	9.57	-213.91	10.96	
18	-1.98	217	-0.872	211	-2.14	8.10	-1.00	9.87	
19	-11.37	217	-10.197	211	-11.28	8.60	-10.52	7.38	
20	-5.35	217	-4.219	211	-6.09	13.77	-4.29	12.89	
21	416.95	221	408.480	215	417.84	13.54	408.76	11.41	
22	353.75	221	346.741	215	354.41	7.83	346.95	11.44	
23	538.03	221	526.777	215	539.68	8.87	527.17	11.65	
24	355.16	221	348.114	215	356.03	9.18	348.39	17.90	

Table 6. Predicted genotypic effects for lint yield (LY, kg/ha) by four methods.

ⁱ: M1 = MINQUE approach without Jackknife; M2 = REML approach without Jackknife; M3 = MINQUE approach with Jackknife; and M4 = REML approach with Jackknife.

with two LMM approaches could significantly reduce standard errors for these estimated variance components and predicted effects and thus statistical power for these parameters increased considerably with the use of jackknife method, as shown in **Table 1**. The results from actual data analysis were highly consistent with the simulated results.

Based on the results from our simulation and actual data analysis in this study, several clear conclusions could be drawn: 1) MINQUE and REML approaches perform equally well (M1 vs M2 and M3 vs M4) regarding variance component estimation and random effect prediction); 2) Jackknife based MINQUE and REML approaches could

	M1	F	M2	!	M	3	M4		
Genotype	Pre	SE	Pre	SE	Pre	SE	Pre	SE	
1	-4.336	2.97	-4.311	2.91	-4.322	0.199	-4.301	0.124	
2	-3.368	2.97	-3.349	2.91	-3.383	0.216	-3.324	0.259	
3	-2.156	2.97	-2.130	2.91	-2.152	0.097	-2.130	0.047	
4	-5.064	2.97	-5.054	2.91	-5.044	0.235	-5.037	0.124	
5	-1.145	2.97	-1.114	2.91	-1.149	0.101	-1.109	0.111	
6	-0.790	2.97	-0.757	2.91	-0.801	0.301	-0.739	0.388	
7	-0.305	2.97	-0.269	2.91	-0.301	0.191	-0.286	0.188	
8	-0.925	2.97	-0.892	2.91	-0.937	0.165	-0.899	0.198	
9	-0.324	2.97	-0.289	2.91	-0.333	0.123	-0.302	0.151	
10	-1.597	2.97	-1.568	2.91	-1.607	0.092	-1.574	0.284	
11	2.455	2.97	2.505	2.91	2.436	0.232	2.487	0.186	
12	1.590	2.97	1.636	2.91	1.600	0.403	1.630	0.305	
13	0.227	2.97	0.265	2.91	0.219	0.112	0.260	0.154	
14	-2.830	2.97	-2.808	2.91	-2.815	0.258	-2.795	0.180	
15	-0.535	2.97	-0.500	2.91	-0.506	0.557	-0.496	0.410	
16	1.263	2.97	1.307	2.91	1.238	0.160	1.303	0.117	
17	-1.967	2.97	-1.940	2.91	-1.969	0.186	-1.931	0.231	
18	-0.840	2.97	-0.807	2.91	-0.850	0.207	-0.806	0.152	
19	0.541	2.97	0.580	2.91	0.539	0.155	0.561	0.155	
20	-1.462	2.97	-1.433	2.91	-1.465	0.131	-1.416	0.263	
21	5.759	3.00	5.589	2.94	5.773	0.097	5.582	0.096	
22	2.465	3.00	2.413	2.94	2.463	0.122	2.406	0.107	
23	7.824	3.00	7.579	2.94	7.844	0.139	7.573	0.104	
24	5.510	3.00	5.349	2.94	5.522	0.091	5.342	0.145	

Table 7. Predicted genotypic effects for lint percentage (LP, %) by four methods.

ⁱ: M1 = MINQUE approach without Jackknife; M2 = REML approach without Jackknife; M3 = MINQUE approach with Jackknife; and M4 = REML approach with Jackknife.

improve test power while maintaining acceptable Type I error (M1 vs M3 and M2 vs M4); and 3) MINQUE approaches provide less computational intensity especially integrated with jackknife approaches or for simulation study compared to REML approaches.

Though, in this study, we only reported results based on a given data set, many other results also showed the similar patterns that we have found in this study. The methods used for simulations and actual data analysis and example R scripts are available in the two R packages, minque and qgtools [23] [24]. Interested readers may follow these R scripts to conduct their own statistical data analysis and model comparisons and evaluations.

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