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Comparison of Iterative Procedures for Solving Equations for Sire Evaluation

L. Dale Van Vleck
University of Nebraska-Lincoln, dvan-vleck1@unl.edu

D. J. Dwyer
Cornell University

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L. D. VAN VLECK and D. J. DWYER
Department of Animal Science
Cornell University
Ithaca, NY 14853

ABSTRACT

Gauss-Seidel, successive overrelaxation, end-of-round relaxation, and block iteration methods of obtaining solutions for sire effects from equations rising from progeny with records in mixed model procedures were compared. Equations transformed to provide direct solutions for genetic group plus sire effects as well as constrained and unconstrained equations were compared also. Equations for milk yield for the Northeast Artificial Insemination Sire Comparison numbered 301 for Ayrshires, 325 for Brown Swiss, 6,010 for Holsteins, and 926 for Jerseys after absorption of herd-year-season effects. Numbers of coefficients were 15 to 20% less for transformed equations, which decreased computing time per round of interation about 15%. Solutions for transformed equations converged more rapidly than solutions for untransformed equations with convergence criterion the ratio of the residual norm to the norm of the right-hand sides. Successive overrelaxation generally was more efficient than Gauss-Seidel iteraton. Solutions for equations constrained to full rank converged more slowly than unconstrained equations. Block iteration was more efficient than single equation iteration.

INTRODUCTION

One obstacle for computing evaluations of sires from records of progeny by mixed model procedures is in solving a large number of equations. The usual procedure when the model includes fixed herd-year-season effects, random sire effects, and random residual effects is to absorb herd-year-season equations into sire equations because herd-year-season solutions usually are not needed. If sires are nested within fixed subpopulations, genetic group equations then are generated from sire equations. The last step in formation of the equations is to add the inverse of the relationship matrix among sires times the ratio of residual to sire components of variance to the diagonal block of coefficients corresponding to sire effects. The resulting mixed model equations then are solved iteratively. The traditional method is Gauss-Seidel (GS) iteration, which is guaranteed to converge if the equations are symmetric and positive definite. With a constraint on the equations to account for the dependency between fixed herd-year-season and group effects, the equations have that property.

Textbooks on numerical analysis (e.g., 3, 4, 5, 8) suggest strongly that other iterative procedures may converge more quickly than GS. The purpose of this study was to compare GS iteration, successive overrelaxation (SOR), GS iteration together with end-of-round relaxation (EOR), constrained and unconstrained equations, a form of block iteration (BLOCK), and successive overrelaxation with transformed equations (QP-SOR). These are only a few of the possible combinations of iterative procedures available, but they are also the ones most likely to be used.

METHODS

Equations after absorption of herd-year-season effects, formation of group equations, and addition of the product of the inverse relationship matrix and the scalar ratio, $\lambda = (4-h^2)/h^2$, where $h^2 = .25$ is heritability for milk evaluations from the January 1982 Northeast Artificial Insemination Sire Comparison (NEAISC), were available for study. The maternal grandsire (MGS) model (1, 6) also includes fixed group effects corresponding to probable year of birth of unknown maternal grandsires.

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The equations, after absorption of herd-year-season equations, can be represented symbolically as:

$$\begin{bmatrix} \mathbf{M'M} & \mathbf{M'S} & \mathbf{M'G} \\ & \mathbf{S'S}+\mathbf{A}^{-1}\lambda & \mathbf{S'G} \\ \text{Symmetric} & & \mathbf{G'G} \end{bmatrix} \begin{bmatrix} \mathbf{m} \\ \mathbf{s} \\ \mathbf{g} \end{bmatrix} = \begin{bmatrix} \mathbf{M'y} \\ \mathbf{S'y} \\ \mathbf{G'y} \end{bmatrix}$$

where:

- **m** is vector of solutions for groups of unknown maternal grandsires,
- **s** is vector of solutions for sire effects including base sires with no daughters that are incorporated because of relationships to bulls with daughters,
- **g** is vector of solutions for fixed group effects, and
- $\mathbf{A}^{-1}$ is inverse of the relationship matrix among bulls and base sires.

The sire comparison for a specified bull is the sum of the sire solution and the solution for his group. Thus, sire comparisons are:

$$\mathbf{Qg} + \mathbf{s}$$

where Q is a matrix that assigns sires to groups.

The QP transformation proposed by Quaas and Pollak (7) results in the same number of equations but with fewer coefficients. They stated that they thought there might be some computational advantage because of increased sparseness but did not expect much difference in computational efficiency. The sire comparison is solved for directly from the transformed equations:

$$\begin{bmatrix} \mathbf{M'M} & \mathbf{M'S} & 0 \\ & \mathbf{S'S}+\mathbf{A}^{-1}\lambda & -\mathbf{A}^{-1}\mathbf{Q}\lambda \\ \text{Symmetric} & & \mathbf{Q'A}^{-1}\mathbf{Q}\lambda \end{bmatrix} \begin{bmatrix} \mathbf{m} \\ \mathbf{Qg}+\mathbf{s} \\ \mathbf{g} \end{bmatrix} = \begin{bmatrix} \mathbf{M'y} \\ \mathbf{S'y} \\ \mathbf{0} \end{bmatrix}$$

Starting Points

That starting points will influence rate of convergence is well known. After preliminary investigation, a choice of starting points that has the approximate expected value of the final solutions seemed to be most appropriate. Consequently for all methods starting points were:

$$\mathbf{g}^0 = (\mathbf{G'G})^{-1}\mathbf{G'y}$$
$$\mathbf{m}^0 = \mathbf{0}$$
$$\mathbf{s}^0 = \mathbf{0}$$

where the superscript denotes the initial (0) round of iteration.

The initial solution for $\mathbf{g}^0$ was obtained by a decomposition method described later rather than by inverting $\mathbf{G'G}$.

Stopping Points

Stopping points for iteration are arbitrary. To standardize for the magnitude of the observations, various fractions of the Euclidean norm of the right-hand side vector were chosen as stopping points.

Let the equations be:

$$\mathbf{Ab} = \mathbf{r}$$

with Euclidean norm, $(\mathbf{r'r})^{.5} = (\Sigma r_i^2)^{.5}$.

The residual from each right-hand side can be approximated as part of the iterative procedure. In most cases this residual will be, on the average, about half a round earlier than if computed at the end of the round. The residual vector at round n is:

$$\mathbf{e}^n = \mathbf{r} - \mathbf{Ab}^n$$

The rule for stopping was when:

$$(\mathbf{e'e})^{.5} \leqslant C(\mathbf{r'r})^{.5}$$

where C is chosen arbitrarily. Three C were chosen: .01, .001, and .0001. Iteration was stopped at 100 rounds whether or not the stopping point was reached. The C of primary interest was .001.

Methods of Iteration

All methods were applied without imposed constraints unless noted as suggested by Stephen P. Smith (1982, personal communication). His theorem is that constraints do not need to be applied to the equations to obtain convergence, and without constraints, solutions probably converge more quickly.

Successive Overrelaxation and Gauss-Seidel

For SOR, the i^{th} solution in round n can be

written:

$$b_i^n = b_i^{n-1} + (w/a_{ii})(r_i - \sum_{j=1}^{i-1} a_{ij}b_j^n - a_{ii}b_i^{n-1} - \sum_{j=i+1}^{N} a_{ij}b_j^{n-1})$$

where w is the relaxation factor ($1 \leq w < 2$) and N is the number of equations. When $w = 1$, SOR reduces to GS iteration. When written in this form, the last term in parentheses is the residual, e_i^n, just prior to obtaining the i^{th} solution for the next round. On the average, e_i^n will be calculated one-half round earlier than if calculated at the end of the round, which would require extra computations.

End-of-Round Relaxation

End-of-round relaxation is the same as GS iteration except that at the end of the round the previous and new vectors of solutions, $\mathbf{b}^{n-1}$ and $\mathbf{b}^{n*}$, are combined to form the solution vector for the n^{th} round:

$$\mathbf{b}^n = \mathbf{b}^{n-1} + w(\mathbf{b}^{n*} - \mathbf{b}^{n-1})$$

Zero Last

A constraint often imposed is to set the last element of the group solution vector to zero (ZERO LAST). Computations are the same as for SOR except for one less equation.

Zero Sum

A common LaGrange multiplier constraint is to force the group solutions to sum to zero (ZERO SUM). Then the constraint equation is:

$$g_1 + g_2 + \ldots + g_L + 0\alpha = 0$$

The corresponding coefficient of α in each group equation is 1 and is 0 for all other equations. The zero on the diagonal of the LaGrange equation prevents use of standard iteration procedures. However, if the LaGrange and last group equation are interchanged, diagonals are nonzero, but the equations are no longer symmetric or positive definite. Successive underrelaxation (SUR with $0 < w \leq 1$) was required to obtain converge. Convergence was obtained only with a limited number of w and only after many rounds of iteration. The procedure was attempted on only Ayrshire equations.

Another idea was to put something on the diagonal of the LaGrange equation, e.g., $g_1 + g_2 + \ldots + g_L + L\alpha = 0$. However, on a small example, the procedure diverged immediately with GS (R. L. Quaas, 1981, personal communication). Therefore, this alternative was not pursued.

Putting the LaGrange multiplier equation into the group equations and using block iteration for the group equations similar to the BLOCK procedure described shortly probably would have worked about as well as the BLOCK procedure but was not thought of until the project was completed.

Subtracting Average Group Solution

R. W. Everett (1981, personal communication) determined that the only constraint he was using was to subtract the average group solution from each of the group solutions (SUB AVE) at the end of a round. R. L. Quaas (1982, personal communication) reasoned that this is such a minor adjustment that it would be essentially the same as no constraint at all. He was correct, as will be demonstrated.

Block Iteration

C. R. Henderson originally solved for all elements of the group solution vector simultaneously in each round (2). This would be BLOCK for the group equations and point iteration for the remaining equations. At that time the traditional view was that a constraint was necessary. Therefore, he probably zeroed out the last group solution and equation or added a LaGrange multiplier equation and obtained an inverse solution after adjusting the right-hand sides for solutions to the other equations. In this study no constraint was used, and in agreement with texts on numerical analysis (3, 4, 5), BLOCK was obtained by a Cholesky decomposition procedure rather than an inverse procedure to save a few seconds of time. In either case, the inverse or Cholesky decomposition needs to be obtained only in the first round and as part of obtaining the starting point for the group solutions.

In terms of an inverse procedure:

$$\mathbf{g}^{n*} = (\mathbf{G}'\mathbf{G})^{-1}(\mathbf{G}'\mathbf{y} - \mathbf{G}'\mathbf{M}\mathbf{m}^{n} - \mathbf{G}'\mathbf{S}\mathbf{s}^{n})$$

where $(\mathbf{G}'\mathbf{G})^{-1}$ is the inverse of $\mathbf{G}'\mathbf{G}$, and:

$$\mathbf{g}^{n} = \mathbf{g}^{n-1} + w(\mathbf{g}^{n*} - \mathbf{g}^{n-1})$$

With the Cholesky procedure $\mathbf{G}'\mathbf{G}$ is decomposed to $\mathbf{L}\mathbf{L}'$ where $\mathbf{L}$ is a lower triangular matrix. Then the equations to be solved are:

$$(\mathbf{L}\mathbf{L}')\mathbf{g}^{n*} = \mathbf{r}^{n*}$$

where $\mathbf{r}^{n*} = (\mathbf{G}'\mathbf{y} - \mathbf{G}'\mathbf{M}\mathbf{m}^{n} - \mathbf{G}'\mathbf{S}\mathbf{s}^{n})$. Next, let:

$$\mathbf{u}^{n*} = \mathbf{L}'\mathbf{g}^{n*}$$

and solve for $\mathbf{u}^{n*}$ from:

$$\mathbf{L}\mathbf{u}^{n*} = \mathbf{r}^{n*}$$

which is easy because the upper off-diagonal elements of $\mathbf{L}$ are zero. The back solution is for $\mathbf{g}^{n*}$ from:

$$\mathbf{L}'\mathbf{g}^{n*} = \mathbf{u}^{n*}$$

which is also easy, because the lower off-diagonal elements of $\mathbf{L}'$ are zero. The last element of $\mathbf{g}^{n*}$ is obtained first.

Finally, as before:

$$\mathbf{g}^{n} = \mathbf{g}^{n-1} + w(\mathbf{g}^{n*} - \mathbf{g}^{n-1})$$

Successive Overrelaxation with Transformed Equations

The QP-SOR transformed equations were solved only by SOR and GS.

RESULTS AND DISCUSSION

Numbers of equations and groups and coefficients for four breeds are in Table 1. The prediction of Quaas and Pollak (7) that the coefficient matrix would be more sparse with transformation was confirmed.

Time required per round of iteration is dependent on the computer and how the equations are stored. In this case nonzero coefficients of equations were stored on immediate access disk with a full equation read into computer memory at a time. Timings in Table 2, however, should be proportional for other computers using a similar access system. Relative times are about as expected from knowledge of equations and procedures. Block iteration theoretically would not take any longer than SOR except for the first round when elements of $(\mathbf{G}'\mathbf{G})^{-1}$ or L are calculated. The computation of $\mathbf{L}$, however, probably results in a more dense coefficient matrix than $\mathbf{G}'\mathbf{G}$ and, therefore, leads to more multiplications per round. There are also a few extra steps in computing the residual vector. Nevertheless, the QP transformed equations appear to require 11 to 15% less time per round as predicted from the smaller number of coefficients.

Ayrshire Equations

Numbers of rounds required for convergence to C = .01, .001, and .0001 for the Ayrshire equations are in Table 3. Results for SOR and QP-SOR are listed first because they turned out to be of most interest.

Successive overrelaxation was much more efficient than GS (w = 1) with the number of rounds saved to the same convergence criterion depending on the convergence criterion and

TABLE 1. Number of equations to be solved, number of fixed genetic groups, and number of nonzero coefficients for the usual mixed model equations and the transformed (QP) equations.

Breed	No. of equations	Fixed genetic groups	Mixed model coefficients	QP coefficients
Ayrshire	301	10	24,446	21,692
Holstein	6,010	56	2,162,110	1,838,538
Jersey	926	32	108,954	85,092
Brown Swiss	325	10	19,088	16,824

TABLE 2. Average central processing unit times (seconds per round) required for various iterative procedures for the Ayrshire and Holstein equations.

	Ayrshire	Holstein
Successive overrelaxation (SOR) and Gauss-Seidel	1.14	91.39
End-of-round relaxation	1.15	91.75
Zero last group solution	1.14	91.31
Subtract average group solution from each group solution	1.14	91.57
Block iteration for group solutions	1.21	97.68
(first round only)	(2.17)	(178.62)
QP transformed equations (SOR)	1.03	77.78

with any of the relaxation factors less than 1.5 was more efficient than GS.

The dramatic result is the reduction of numbers of rounds required with QP transformed equations. Only one-third to one-half as many rounds were required depending on C. In only a few cases was any QP-SOR procedure less efficient than the best SOR.

The combination of SOR with block iteration for the group vector and point iteration for the others was generally superior to SOR alone and was relatively more efficient for more rigorous stopping criteria. The optimum relaxation factor for BLOCK-SOR appeared to be larger than for SOR.

Other convergence criteria also were computed but have not been summarized. If the

TABLE 3. Number of rounds* to reach specified convergence criteria for Ayrshire sire equations.

Convergence criterion (C)	Relaxation factor (w)									
	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9
					Successive overrelaxation (SOR)					
.01	18	16	15	15	16	18	19	21	23	39
.001	43	36	32	32	33	35	40	39	44	85
.0001	70	54	51	49	50	53	58	55	67	*
					QP transformed – SOR (QP-SOR)					
.01	10	9	8	7	7	8	9	12	19	37
.001	27	22	19	15	12	11	14	20	29	60
.0001	45	37	30	24	18	15	20	27	41	82
					Block on groups, point on others (BLOCK)					
.01	24	21	19	17	15	13	12	18	24	46
.001	55	46	38	31	25	23	25	30	40	82
.0001	87	71	58	45	35	34	37	43	59	*
					End-of-round relaxation (EOR)					
.01	18	16	15	14	13	12	12	16	32	*
.001	43	38	36	33	31	29	27	27	52	*
.0001	70	64	58	54	50	46	43	41	69	*
					Zero last group solution (ZERO LAST)					
.01	17	16	15	15	16	24	31	35	38	61
.001	77	64	71	67	62	55	48	63	86	*
.0001	*	*	*	*	*	85	67	91	*	*
					Subtract average group solution from each group solution (SUB AVE)					
.01	18	16	15	15	16	17	20	22	23	36
.001	43	36	32	32	34	36	41	47	49	65
.0001	70	54	51	50	51	51	61	68	70	88

*Indicates more than 100 rounds.

convergence criterion is maximum change from round to round for any solution, there is an indication that the advantage of the QP transformation is not as great as when the convergence criterion is the norm of the residual vector.

End-of-round relaxation with an optimum relaxation factor was more efficient than SOR. The efficiency of the EOR procedure appears to be more dependent on the convergence criterion and relaxation factor than SOR. Convergence by 100 rounds for w = 1.9 was not achieved with EOR even to C = .01 but was achieved for SOR to C = .001. Textbooks do not mention EOR. Smith (1982, personal communication) reports that EOR is guaranteed to converge if SOR is guaranteed to converge.

As Smith predicted, applying a constraint generally required more rounds to converge than with no constraint, especially for smaller C. These results are supported by similar observations (H. T. Blair, J. I. Weller, and K. Agyemang, personal communication, 1982).

As Quaas predicted, SUB AVE at the end of a round was essentially the same as applying no constraint over a wide range of relaxation factors. However, SOR with no constraint was more efficient for C = .001 and .001 for w = 1.6, 1.7, and 1.8 but was less efficient for w = 1.9 than SOR with the SUB AVE constraint.

The results for the sum to zero constraint when the LaGrange equation was switched with the last group equation are not shown. Convergence to C = .01 was achieved in 65, 38, and 31 rounds for w = .3, .5, and .6. Convergence to C = .0001 was achieved in 187 rounds for w = .6. With w = .7 and 1.0, the solutions diverged after the first round. This procedure is not recommended, but a form of block iteration maintaining symmetry of the equations probably would converge, although more slowly than when no constraint is imposed.

Holstein Equations

Because the Holstein equations took about 3 h of computer time for 100 rounds of iteration, the strategy generally was to choose what might be an optimum relaxation factor based on Ayrshire, Jersey, and Brown Swiss results and then change relaxation factor until the minimum number of rounds of iteration for each convergence criterion was found.

Results for Holstein equations are in Table 4. In most cases only convergence to C = .01

TABLE 4. Number of rounds[1] to reach specified convergence criteria for Holstein sire equations.

Convergence criterion (C)	Relaxation factor									
	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9
					Successive overrelaxation (SOR)					
.01	29	29	31	34	36	39	44	51		
.001	*	*	*	*	*	*	(*)	*		
					QP transformed-SOR (QP-SOR)					
.01				11	9	9	10	14		
.001				19	17	17	17	20		
.0001				28	27	25	25	30		
					Block on groups, point on others (BLOCK)					
.01						30	29	29	35	
.001						97	83	73	70	
.0001						*	*	(*)	*	
					End-of-round relaxation (EOR)					
.01						19	18	18	26	81
.001						*	*	*	(*)	*

*Indicates more than 100 rounds.

(*)Indicates smallest residual norm at 100 rounds relative to other relaxation factors.

was possible within 100 rounds. In those cases, the relaxation factor with smallest squared residual at 100 rounds is indicated. The pattern is similar to that for Ayrshire equations. Iteration with successive overrelaxation of the QP equations was most efficient and was the only procedure to converge for C = .0001 by 100 rounds. A relaxation factor of 1.3 to 1.5 seems nearly optimum for both breeds with the QP equations.

The block procedure allowed convergence to C = .001 by 100 rounds.

The EOR procedure appeared much more efficient than SOR for C = .01. The optimum w for C = .01 was also larger for EOR than SOR. Neither procedure converged for C = .001 in less than 100 rounds. The norm of the residual vector, however, was only 50% as large for SOR with optimum w = 1.6 as for EOR with optimum w = 1.8 at 100 rounds, again suggesting that EOR is relatively less efficient for more rigorous convergence criteria.

The results for the other breeds suggested that ZERO LAST, ZERO SUM, and SUB AVE were not likely to be better than SOR, EOR, or QP-SOR, so those procedures were not studied for Holstein equations.

Jersey and Brown Swiss Equations

Jersey and Brown Swiss results are summarized in Tables 5 and 6. Only relaxation factors associated with fewest rounds of iteration are reported. The patterns are again similar.

CONCLUSIONS

Generalization of results to other sets of equations may not be appropriate. A general rule in use of iterative procedures is that what works best for one set of equations might not be best for another set of equations. For similar sets of sire evaluation equations, similar results however, might be expected and at least, could be used as guidelines.

The main conclusions are as follows: 1) Successive overrelaxation was more efficient than GS iteration for a wide range of relaxa-

TABLE 5. Relaxation factors with smallest number of rounds of iteration required to meet convergence criteria for different iterative procedures for Jersey sire evaluation.

Procedure	Convergence criterion (C)	Optimum relaxation factor (w)	No. rounds required
Successive overrelaxation (SOR)	.01	1.5, 1.6	16
	.001	1.4, 1.5	35
	.0001	1.4	50
QP transformed with SOR (QP-SOR)	.01	1.4, 1.5	9
	.001	1.5	14
	.0001	1.5	20
Block iteration on groups (BLOCK)	.01	1.5, 1.6	16
	.001	1.6	25
	.0001	1.5, 1.6	46
End-of-round relaxation (EOR)	.01	1.6, 1.7	16
	.001	1.7	37
	.0001	1.7	60
Zero last group solution (ZERO LAST)	.01	1.4, 1.5	17
	.001		*
	.0001		*
Subtrait average group solution from each group solution (SUB AVE)	.01	1.5, 1.6	16
	.001	1.4, 1.5	35
	.0001	1.4	51

*Indicates more than 100 rounds required.

TABLE 6. Relaxation factors with smallest number of rounds of iteration required to meet convergence criteria for different iterative procedures for Brown Swiss sire evaluation.

Procedure	Convergence criterion (C)	Optimum relaxation factor (w)	No. rounds required
Successive overrelaxation (SOR)	.01	1.1, 1.2, 1.3	11
	.001	1.3, 1.4	19
	.0001	1.3	25
QP transformed with SOR (QP-SOR)	.01	1.5, 1.6	13
	.001	1.5	17
	.0001	1.5	29
Block iteration on groups (BLOCK)	.01	1.3, 1.4, 1.5	10
	.001	1.5	14
	.0001	1.5	19
End-of-round relaxation (EOR)	.01	1.4	9
	.001	1.6	19
	.0001	1.6	28
Zero last group solution (ZERO LAST)	.01	1.5, 1.6	14
	.001	1.5	20
	.0001	1.6	32
Subtrait average group solution from each group solution (SUB AVE)	.01	1.2	10
	.001	1.3, 1.4	19
	.0001	1.3	25

tion factors. 2) Adding traditional constraints – zeroing out an equation or forcing solutions to sum to zero – to obtain full rank equations slowed convergence. 3) Henderson's original method of block iteration for the fixed (group) equations and single equation iteration for sire equations was more efficient than single equation iteration for all equations. 4) Iteration of the QP transformed equations was not only faster per round of iteration, but many fewer rounds of iteration were required to reach the same precision measured as a ratio of the residual norm to the norm of the right-hand sides.

The QP transformed equations generally solved most efficiently with SOR except with the Brown Swiss equations. The optimum SOR, EOR, and BLOCK procedures were slightly more efficient than QP-SOR for Brown Swiss equations.

The disturbing result was that the optimum relaxation factor for SOR was different for all breeds. The original hope was that the same factor would be best for all breeds.

The results with QP-SOR, however, are more reassuring. Because of the generally greater efficiency of QP-SOR, that procedure seems to be the method to use. For all breeds a relaxation factor of about 1.5 is indicated. The time per round is also the least because the number of coefficients is smaller. Another advantage of QP is that the sire comparison comes out directly and is easier to save as a starting point when more data are added in future runs.

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