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A Variance Component Estimation Method for Sparse Matrix Applications

James R. Lucas

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PREFACE

This report describes a course of investigation that was pursued by the author while searching for an efficient method for estimating weighting factors to be employed in the adjustment of leveling networks. After the report had been prepared for publication, it was brought to the author's attention that the method described herein had already been published by Forstner (1979a and 1979b) and the convergence of iterated MINQUE and Forstner's estimator to the same estimates had been proven by Schaffrin (1983). Since all three of these references are in German, NGS decided to publish this report in its original form, with this explanatory note and the inclusion of these three references.

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A VARIANCE COMPONENT ESTIMATION METHOD FOR SPARSE MATRIX APPLICATIONS

James R. Lucas
National Geodetic Survey
Charting & Geodetic Services, National Ocean Service
National Oceanic and Atmospheric Administration
Rockville, Md. 20852

ABSTRACT. Methods for estimating variance components from the observation data used in a least squares adjustment are becoming important in geodesy because of the variety of data that need to be combined into a single adjustment. Unbiased estimators of the MINQUE (Minimum Norm Quadratic Unbiased Estimation) type have received the most attention, but these estimators have some shortcomings that make them unattractive in certain applications. In particular, they require the full inverse of the least squares normal equation matrix, thus limiting the use of sparse matrix methods so common to geodesy. This report proposes an iterative estimation method, which may not be unbiased, but produces reliable estimates in controlled numerical tests and is compatible with sparse matrix adjustments. Some results are presented which compare this estimator with MINQUE and iterated MINQUE when applied to a particular adjustment problem.

INTRODUCTION

In recent years the geodetic community has become increasingly interested in methods of estimating variance components. This interest has been stimulated, in part, by a continually expanding need to merge into a single adjustment observations acquired by a variety of instrument systems. There is also a requirement for combining observation data acquired many years, or even decades, ago with modern observations in order to determine crustal motions. Since the technology employed in acquiring observations has been far less static than the quantities being observed, and the displacements are of about the same order of magnitude as observation errors, the weights assigned to these data must be chosen carefully. Estimation of components of variance from the observation data is one of the avenues being explored in an attempt to develop more realistic weighting factors for geodetic adjustments.

At the National Geodetic Survey (NGS), numerical investigations into variance component estimation were begun by the author using MINQUE, as proposed by C. R. Rao (1971a). This method was tested in several different types of adjustments and found to produce estimates that were quite adequate. It seemed reasonable to assume, however, that MINQUE should be initiated with the best available estimates, even if those estimates were obtained from a previous MINQUE. This led to experimentation with iterated MINQE, so designated by Rao because the property of unbiasedness may be lost in the iteration process. If such losses did occur, they did not appear to contaminate the estimates, which improved substantially in most cases.

Prior to these numerical tests, a simpler estimation method had been derived by a colleague, Allen J. Pope. This proved to be an independent derivation of AUE (Almost Unbiased Estimation) proposed by Horn et al. (1975), but Pope had the foresight to suggest that iterated AUE and iterated MINQE should converge to the same set of estimates, though by different paths. His prediction was found to be correct, but we have been unsuccessfull, so far, in formulating a general statement of the conditions for which it is true.

Iterated AUE requires only a fraction of the computer storage consumed by MINQUE, and far less computation than iterated MINQE, even though it usually requires more iterations to converge to the same degree of approximation. Its primary advantage to geodesists, however, is its compatibility with the sparse matrix techniques generally used in geodetic adjustments. MINQUE and, therefore, iterated MINQE are computed from the full inverse of the least squares normal equation coefficient matrix. If no advantage is gained from the sparse systems of equations encountered in geodesy, then MINQUE estimates are very expensive to compute.

MINQUE

C. R. Rao (1971a, 1971b, 1972) provides a thorough and elegant derivation of MINQUE. He begins with the assumption that a linear function of the variance components in a general linear model can be estimated from a quadratic function in the observables. He then proceeds to show that minimization of a particular matrix norm, employing the constraints of unbiasedness and invariance with respect to translations of the parameter vector, leads to a set of estimating equations that is MINQUE.

The following paragraphs are included to provide some of the background for MINQUE and to establish a set of notation, which is different from that used by Rao. It is hoped that this material will provide sufficient background information for those readers not familiar with variance component estimation methods. However, it is recommended that such readers, with more than a casual interest in the subject, refer to one or more of the excellent papers by C. R. Rao.

Consider the linear model

$$Y = AX + U\gamma$$
$$= AX + U_1\gamma_1 + \ldots + U_k\gamma_k \qquad (1)$$

where Y is an n vector of observations, A is a given n by p matrix, X is a p vector of unknown parameters, U_i is a given n by c_i matrix, and γ_i is a c_i vector of random errors such that

$$E(\gamma_i) = 0$$
$$E(\gamma_i\ \gamma_i^T) = \sigma_i^2\ I \qquad (2)$$
$$E(\gamma_i\ \gamma_j^T) = 0 \quad (i \neq j)$$

where E is the expected value operator, and the σ_i^2 are unknown variance components to be estimated along with the parameter vector X.

From eqs. (1) and (2) the expectation of Y is AX and its dispersion matrix is

$$D(Y) = \sigma_1^2\ V_1 + \ldots + \sigma_k^2\ V_k$$

where

$$V_i = U_i\ U_i^T.$$

Let α_i^2 be an a priori estimate of σ_i^2. In the unusual case of complete ignorance of even the magnitudes of the variance components, we can let all a priori estimates be unity. In either case, the weight matrix

$$W = H^{-1}$$

where

$$H = H_1 + \ldots + H_k$$

and

$$H_i = \alpha_i^2\ V_i \qquad (3)$$

is used to obtain the least squares estimate for the unknown parameters

$$\hat{X} = (A^T\ W\ A)^{-1}\ A^T\ W\ Y$$
$$= N^{-1}\ A^T\ W\ Y \qquad (4)$$

and the matrix

$$R = W - W\ A\ N^{-1}\ A^T\ W. \qquad (5)$$

From eq. (5) it can be seen that RA = 0 and, therefore,

$$RY = R(AX + U\gamma) = RU\gamma. \tag{6}$$

With this result, we can construct k equations of the form

$$\begin{aligned} E(Y^T R V_i R Y) &= E(\gamma^T U^T R V_i R U \gamma) \\ &= \sigma_1^2 \operatorname{tr}(U_1^T R V_i R U_1) + \ldots \\ &\qquad + \sigma_k^2 \operatorname{tr}(U_k^T R V_i R U_k) \\ &= \sigma_1^2 \operatorname{tr}(R V_i R V_1) + \ldots \\ &\qquad + \sigma_k^2 \operatorname{tr}(R V_i R V_k) \end{aligned} \tag{7}$$

where tr denotes the trace of the matrix or matrix products. Hence an unbiased estimate of the variance components vector can be obtained from

$$S \hat{\sigma} = q \tag{8}$$

where

$$S_{ij} = \operatorname{tr}(R V_i R V_j)$$

$$q_i = Y^T R V_i R Y$$

and the result is MINQUE of the variance components.

ALTERNATIVE ESTIMATORS

There are three deficiencies of MINQUE which may be important in particular problems: 1) MINQUE sometimes produces variance component estimates that are negative, 2) the S matrix of eq. (8) may be singular in some problems, and 3) MINQUE is expensive to compute for large adjustment problems.

Negative estimates may be valuable in the investigation of random error sources of a class of adjustments. If variance component estimates are obtained from many sets of observation data to compute a set of means, then negative estimates may be meaningful contributions to the means, but in terms of a particular adjustment the occurrence of negative estimates creates a troublesome situation. It has been suggested that the negative estimates be replaced by zero or by small positive quantities, based on the assumption that the true values are insignificantly different from zero.

Rao and Kleffe (1979) treat the possibility of negative estimates in an investigation of MINQE(U,D)--minimum norm estimators that are both unbiased and non-negative definite. They conclude that such estimators exist for some cases, but not the general problem, which explains why estimators which avoid the deficiencies of MINQUE are derived by dropping or relaxing the condition of unbiasedness.

The third deficiency, the cost in computer time and storage of obtaining MINQUE for very large observation sets, is perhaps the most important in geodetic applications. The matrix R is of order n, the number of observations, and constructing it explicitly requires all elements of the inverse of the least squares normal equation matrix. In most geodetic adjustments the normal equations are sparse, and this sparseness is exploited in covariance propagation so that only a small subset of the elements of the inverse need be computed. Hence, computing the full inverse, forming the matrix R, and evaluating the traces of a number of matrix products (that contain R twice) adds a tremendous amount of computation to an already large adjustment problem.

Horn et al. (1975) propose an estimator that they call AUE (Almost Unbiased Estimator), which avoids the deficiencies of MINQUE and is unbiased, provided that the a priori estimates are proportional to the true variances. Considered in terms of practical applications, this condition seems to create a paradox. Seldom, if ever, will this condition be satisfied in a practical application and, if it were, the need for variance component estimates would have vanished because the proportionality factor can be estimated as a variance of unit weight. The authors point out, however, that the bias introduced by failure to meet this condition can be expected to be small. Hence, the appellation "almost unbiased."

If $\sigma_i^2 = f\ \alpha_i^2$ for all i, then a slight modification of (7) produces

$$E(Y^T R H_i R Y) = f\ \alpha_i^2 [\ tr(R V_i R H_1) + \ldots + tr(R V_i R H_k)\ ]$$
$$= \sigma_i^2\ tr(R V_i R H). \quad (9)$$

From the definition of R, eq. (5), it can be seen that the product RH is an idempotent matrix. Hence, RHR = R and $tr(R V_i R H) = tr(R V_i)$, which produces the estimator

$$\hat{\sigma}_i^2 = (Y^T R H_i R Y)/tr(R V_i) \quad (10)$$

which is AUE.

The denominator in eq. (10) is the sum of all elements in the i-th row (or column) of S, each of which has the form

$$tr(R V_i R V_j) = tr(R U_i U_i^T R U_j U_j^T)$$
$$= tr[(U_i^T R U_j)(U_i^T R U_j)^T]$$

which is a sum-of-squares. Hence, all elements of S are non-negative and eq. (10) is a non-negative estimator of the variance components.

AUE is biased for all practical applications, though this bias may be small if the a priori values are approximately proportional to the true variance. It can be shown that AUE tends to produce estimates that are somewhere between the true variances and the mean of the true variances, i.e., large variance components are underestimated while small ones are overestimated.

ITERATIVE ESTIMATION

Although MINQUE provides an unbiased estimate of the variance components, MINQUE is not unique in that the estimates are subject to some variation depending upon the prior values. This dependence on prior values leads to some lack of confidence in estimates that are significantly different from the a priori values. Would better initial approximations produce better estimates? If MINQUE estimates are used to initiate a second MINQUE, will the results be closer to the true variance?

Rao (1972) suggests the possibility of iterating MINQUE, but warns that the property of unbiasedness will usually be lost. He concedes that such estimates may have other interesting properties which have yet to be investigated.

Iteration raises some difficult questions for the theoretician. Conditions under which the iteration converges must be explored, and the bias (or lack thereof) is much more difficult to access. But, if one is concerned with variance component estimation as a means of improving the weighting factors employed in a least squares adjustment, iteration can be justified by the end result. When the iteration converges, assuming that it does, the computed variance component estimates will be the same as those used in the least squares adjustment. Intuitively, it is difficult to believe that such consistency could result from poorer estimates of the true variances than could be obtained with a priori values chosen by guess.

Numerical experiments with simulated data indicate that iteration sometimes improves the MINQUE estimates and sometimes does not, but whenever there is significant change with iteration, it is in the direction of the true values. While it is dangerous to generalize from a small number of experiments, it appears that iteration is not likely to contaminate the estimates and has the potential for improving them significantly.

These experiments produced another result that was quite interesting. In all cases, except one, in which MINQUE produced a negative estimate for one or more of the variance components, these estimates became and remained positive after one or two iterations. The only exception was a case in which the S matrix in the estimating equations was very ill-conditioned. Hence, unlike MINQUE, iterated MINQE is not likely to produce negative estimates. However, the already substantial computing task required by MINQUE is increased by a factor of at least two with iteration.

Since the property of unbiasedness may be lost anyway, the simpler AUE estimator is an advantageous alternative when employed in an iterative process. Rather than assuming a single proportionality constant, as in the derivation of AUE, we use a separate unknown variance factor for each variance component. With this modification eq. (9) can be written as

$$E(Y^T R H_i R Y) = \sigma_1^2 \operatorname{tr}(R H_i R V_1) + \ldots + \sigma_k^2 \operatorname{tr}(R H_i R V_k)$$
$$= f_1 \operatorname{tr}(R H_i R H_1) + \ldots + f_k \operatorname{tr}(R H_i R H_k) \quad (11)$$

From the idempotency of RH,

$$\operatorname{tr}(R H_i R H_1 + \ldots + R H_i R H_k) = \operatorname{tr}(R H_i) \quad (12)$$

and eq. (11) is unchanged when written in the form

$$E(Y^T R H_i R Y) = \sum_{j=1}^{k} f_j \operatorname{tr}(R H_i R H_j) + f_i \operatorname{tr}(R H_i) - f_i \sum_{j=1}^{k} \operatorname{tr}(R H_i R H_j)$$

$$= f_i \operatorname{tr}(R H_i) + \sum_{j=1}^{k} (f_j - f_i) \operatorname{tr}(R H_i R H_j) \quad (13)$$

Hence, the AUE of the variance factor, rather than the variance component, can be written

$$f_i \approx (Y^T R H_i R Y)/\operatorname{tr}(R H_i) \quad (14)$$

which provides an estimating equation of the form of eq. (8), but with a diagonal coefficient matrix requiring the traces of simpler matrix products.

Equation (14) may be a crude approximation if the initial estimates are not nearly proportional to the true values, as assumed in the derivation of AUE. However, the bias terms are fractions (usually small) of differences between variance factors. Upon iteration, all estimates of the variance factors approach unity and the bias terms, given in the summation, vanish. The rate of convergence will obviously depend on the initial estimates, but a choice of unity for all starting values produces satisfactory estimates after a few iterations.

IAUE (Iterated AUE) will not produce negative estimates and does not require the matrix S. But a more significant advantage is its facility with sparse matrix adjustments.

In nearly all geodetic adjustments the weight matrix is either diagonal or block diagonal. This allows the observation equations to be partitioned according to the dimensions of the diagonal blocks of H and processed in batches so that computer storage is substantially reduced. Furthermore, the normal equation coefficient matrix is usually sparse so that the pertinent covariance elements are obtainable without inverting the whole matrix.

Consider the matrix equation

$$\begin{bmatrix} -H & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} Z \\ X \end{bmatrix} = \begin{bmatrix} Y \\ 0 \end{bmatrix} \tag{15}$$

The solution produces

$$X = N^{-1} A^T W Y,$$

the least squares estimate for the unknown parameters, and

$$Z = -W Y + W A X = -R Y,$$

the vector of weighted residuals. If this vector is computed an element at a time, or using whatever partitioning was employed in forming the normal equations, the quadratic forms required for AUE can be accumulated an observation at a time, if the H are diagonal.

The inverse of the coefficient matrix in eq. (15) is found to be

$$\begin{bmatrix} -H & A \\ A^T & 0 \end{bmatrix}^{-1} = \begin{bmatrix} -R & W A N^{-1} \\ N^{-1} A^T W & N^{-1} \end{bmatrix}. \tag{16}$$

Assume that this inversion is accomplished using the same partitioning employed in forming the normal equations. This procedure is relatively inexpensive, but will produce only the diagonal blocks of R that correspond to the nonzero elements of the diagonal blocks of H. These are, however, the only submatrices of R that are needed to compute denominator of eq. (14). If the weight matrices are diagonal, only the diagonal elements of R need be computed and the indicated traces can be computed as summations of scalar products.

TEST RESULTS

Iterated MINQE and IAUE have been tested on a variety of small adjustment problems using both real and simulated data. Simulated data that have been contaminated by errors taken from populations with known variances provide a simple means of evaluating the estimates obtained. An interesting example is a simulated leveling network illustrated in figure 1. This network is assumed to have been observed initially along the 80 dotted line segments at a level of precision represented by a variance of 1.0. Densification of the network is assumed to have consisted of observations along the 64 dashed line segments with a variance of 0.01, and finally the 48 solid segments were reobserved with a variance of 0.0001.

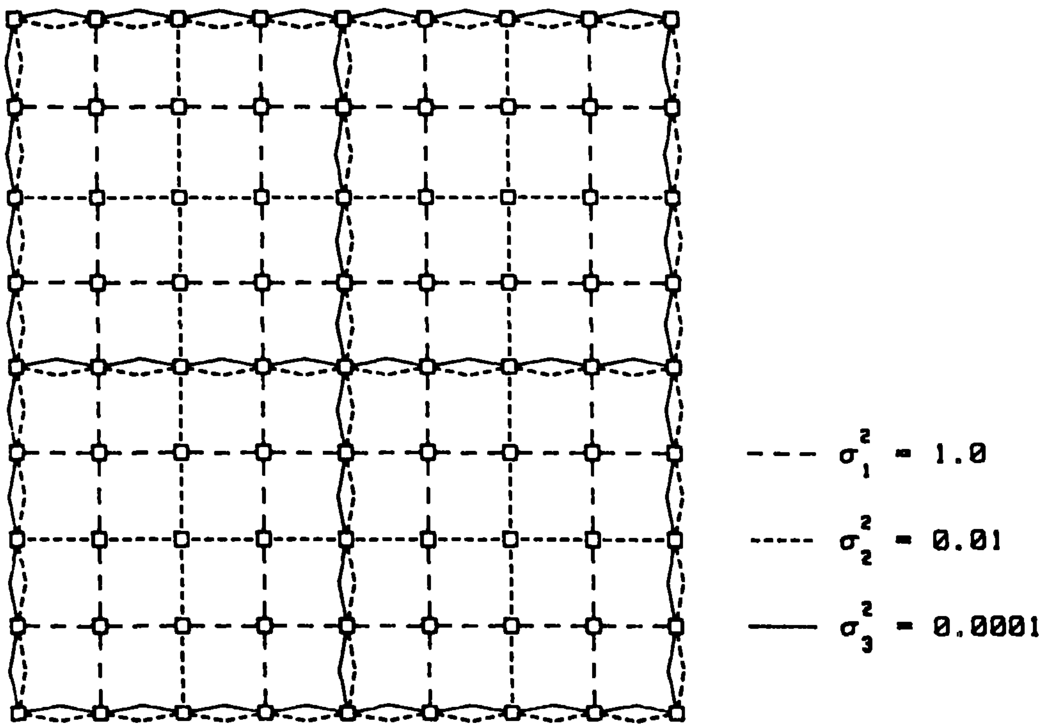

Figure 1.--Simulated leveling network observed in three stages.

Ten sets of simulated data were constructed by adding to each true elevation difference a computer generated random error from a population with zero mean and specified variance. The spread in the variance components was chosen to be large in order to test the ability of IAUE to converge under difficult circumstances. As mentioned previously, each iteration of IAUE tends to underestimate the spread among the corrections to the estimates, so a large spread in the true values might inhibit convergence.

These data sets were used to estimate the variance components in two different computer programs: one which uses the method of iterated MINQE and one which computes IAUE using the sparse matrix method described in the previous section. In every case a priori estimates of unity for all three variance components were used to initiate the iteration process. Hence one program produced both MINQUE (the first iteration) and iterated MINQE, while the other produced AUE and IAUE. It is not correct to consider the initial estimates from the IAUE program to be AUE estimates, because the starting values in this test do not reflect any a priori knowledge of the relative magnitudes of the variance components. These columns are included to show that IAUE required considerable correction between the first and last iteration and to emphasize that AUE should not be used without iteration unless good starting values are available.

In this test, as in all others conducted, the two iterative methods converged to the same set of estimates and are, therefore, listed in table 1 under a single heading. All methods obtained the correct order of magnitude of the largest variance component in all cases. In estimating the two smaller variance components, MINQUE produced at least one negative estimate in eight of the ten tests and two negative estimates in four of them. All negative estimates became non-negative after a few iterations, however, and finally converged to the correct order of magnitude for both of the smaller variance components.

Table 1.--Comparison of variance component estimation methods

Data Set	MINQUE σ_1^2	MINQUE σ_2^2	MINQUE σ_3^2	AUE σ_1^2	AUE σ_2^2	AUE σ_3^2	Iterated σ_1^2	Iterated σ_2^2	Iterated σ_3^2
1	.981	-.0384	.04505	.695	.153	.277	.981	.0084	.000088
2	.920	.0274	-.05587	.644	.185	.189	.931	.0072	.000181
3	.668	.0857	.00042	.482	.186	.176	.783	.0056	.000024
4	.702	-.0348	.05424	.500	.105	.212	.721	.0071	.000023
5	.938	-.0030	-.08866	.647	.163	.178	.829	.0073	.000080
6	1.109	-.0115	-.02336	.777	.192	.265	1.039	.0086	.000094
7	.764	-.0071	-.00232	.538	.134	.192	.776	.0103	.000084
8	.914	-.0409	-.04930	.631	.133	.196	.801	.0076	.000020
9	.512	.0071	.12099	.382	.107	.212	.659	.0081	.000063
10	.858	.0111	-.14144	.583	.155	.123	.729	.0042	.000057

While the two iterative methods converged to the same sets of estimates, there was a large difference in the number of iterations required. Table 2 compares the iteration by iteration estimates for the first data set to show the difference in convergence rate between the two. The criterion for terminating the iteration process in both programs required that the change in all estimates be less than one-half of one percent. In general, IAUE required nearly twice as many iterations as iterated MINQE, but only about one-fourth as much computer time and far less storage.

Table 2.--Iteration by iteration comparison of two iterative methods to show difference in convergence rates.

Iteration	Iterated MINQE σ_1^2	Iterated MINQE σ_2^2	Iterated MINQE σ_3^2	IAUE σ_1^2	IAUE σ_2^2	IAUE σ_3^2
1	.981	-.03841	.0450531	.695	.15315	.2765445
2	.610	-.03720	.0599775	.810	.03804	.1052998
3	.964	-.00024	.0085755	.916	.01002	.0236599
4	.990	.01086	-.0054678	.975	.00709	.0051580
5	.903	.01241	-.0002519	.985	.00695	.0021736
6	.981	.00832	.0000858	.984	.00739	.0010319
7	.981	.00836	.0000877	.983	.00782	.0004278
8				.982	.00814	.0001591
9				.982	.00831	.0000942
10				.981	.00835	.0000881
11				.981	.00836	.0000877
Population	1.000	.01000	.0001000	1.000	.01000	.0001000
Sample	1.018	.00756	.0000910	1.018	.00756	.0000910

This simulated adjustment produced more negative estimates from MINQUE than most of the numerical tests conducted and should not be considered a typical example. It was included to show that such results do occur. At the same time, and probably for the same reason --the large spread in variance component magnitude--both iterative methods required more than the usual number of iterations. In most tests with both real and simulated data, iterated MINQE converged in three or four iterations while IAUE required five or six.

CONCLUSION

IAUE provides a convenient method of estimating variance components in sparse matrix adjustments. Because it can be employed without computing the full inverse of the normal equation coefficient matrix, it requires less storage than MINQUE and less computation that iterated MINQE.

Since the regions of convergence have not been established, there is always the possibility of encountering problems for which IAUE fails to converge, but there are indications that such problems will also cause trouble for MINQUE, either in lack of convergence or in negative estimates that fail to become positive. Therefore, IAUE provides an efficient alternative to MINQUE for sparse matrix applications.

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