HUNGARIAN JOURNAL
OF INDUSTRIAL CHEMISTRY
VESZPRÉM
Vol. 29. pp. 67 – 70 (2001)

LEAST SQUARES AND THE MATRIX RICCATI EQUATION

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Received: July 26, 2001

There are a number of methods for least squares and total least squares solution of linear equations. One such method involves solving an appropriate algebraic matrix Riccati equation. This approach is investigated here using an algorithm based on Newton's method with an infinite series solution of the resulting linear matrix equations. Some numerical examples, from the recent literature, are used to illustrate the techniques.

Keywords: Matrix Riccati equation; Newton's method; infinite series solution; overdetermined linear systems; least squares and total least squares.

Introduction

When a system of linear equations

$$LX = M \tag{1}$$

with *L* and *M*, m x n and m x p matrices respectively, does not have a unique solution *X* it is usual to seek a solution that is "best" in some sense by imposing appropriate constraints. This paper is concerned with computing the least squares (LS) solution, which imposes the constraint that X should minimize the norm $\|LX - M\|_E^2$, and the total least squares (TLS) solution which requires X to minimize $\|L-V\|_E^2 + \|M - W\|_E^2$ subject to the constraint

$$VX = W. \tag{2}$$

The main difference between LS and TLS is that the former assumes the matrix *L* is exact whereas the latter allows for errors in both *L* and *M*. Perhaps the most important approach in solving these problems is singular value decomposition (SVD) the use of which is fully discussed in [1] and [2] for LS and TLS respectively. Another possible approach is the following. By using Lagrange multipliers, in the usual way, it can be shown [3], [4], that *X* satisfies the algebraic matrix Riccati equation (AMRE)

$$XM^TLX + L^TLX - XM^TM - L^TM = 0. \tag{3}$$

When Newton's method is applied to the general AMRE

$$XPX + QX + XF + G = 0 \tag{4}$$

a linear matrix equation, solutions X_i of which converge to *X* the solution of Eqn. (4) under appropriate conditions, is obtained. There are many possible ways of solving this linear matrix equation (see, e.g., [5]) and one of these, which involves infinite series, is studied in [6]. Methods for offsetting the difficulties involved if a poor starting approximation is made to the solution and for accelerating convergence are also investigated in [6]. The solution techniques are implemented by two algorithms, *A1* and *A2*, depending on whether *X* is unsymmetric or symmetric. A simplified form of *A1* is given in the Appendix for convenience.

The aim of the present paper is to illustrate the use of *A1* in solving LS and TLS problems by means of a number of numerical examples from the literature.

Numerical Results

Example 1

The first example is taken from [7] and is concerned with modelling the biological activity of fifteen different compounds with respect to a set of eight variables which describe the various morphological and physiochemical properties of the compounds. The data used is given in Table 1 of [7]. Setting the initial approximation $X_0 = 0$ in A1 gave the same least squares solution as in [7] (when rounded),

$$X_{LS} = [0.636, 0.080, 0.095, -0.308, 0.169, 0.241, 0.278, 0.238]^T$$

and, of course, the same value, 0.61, for the residual sum of squares SS. X_{LS} also agrees with L^+M where L^+ is the pseudo-inverse of L.

The smallest singular value of L is 0.337365 and of $[L;M]$ is 0.335713 so that conditions for a unique TLS solution, [2], are (just) satisfied. If A1 is now continued from the solution X_{LS} given above it converges to

$$X = [0.716, 0.259, 0.124, -0.336, 0.186, 0.531, -0.435, 0.337]^T$$

with e = 0.16 before accuracy begins to deteriorate. (Using a line search shows a slight improvement in accuracy before deterioration.) When this model is applied to the whole of the data the resulting sum of squares is 41.893 .

The smallest singular value of $[L;M]$, for this example, is as given above and the SVD formula

$$X = \left[L^T L - (0.335713)^2 I_3\right]^{-1} L^T M$$

gives

$$X = [-4.28, 1.20, -2.21, -1.29, -2.36, 11.00, -14.60, 2.10]^T$$

which has a residual error $e = 6(-4)$ and which is much better than the previous result from A1. If now, however, the above X is used as the starting approximation in A1 the result is refined to give a better X with a residual error less than 10(-6).

Algorithm A1 was also used to compute the sums of squares, denoted by "PRESS" in [7], for both LS and TLS; these measure the predictive properties of the models used. The same groupings of the date were used as in [7] and Table 1 shows the results obtained.

Table 1 Predictive Sums of Squares for Example 1

	Group 1	Group 2	Group 3	Total
LS	1.172	1.183	0.804	3.159
TLS	1.319	1.540	34.832	37.691

The total for LS agrees with that given in [7]. The total for TLS is inflated by the very large value from Group 3 and presumably accounts for the comment, "when full rank is approached, it behaved differently," made regarding TLS in [7] and for the use of rank 3 TLS rather than full rank. (Before making the calculations all the nine sets of data were scaled to have zero mean and unit variance.)

Example 2

This example is taken from [1] and involves finding a linear fit to data given in Table 26.1 in that reference. In [1] five different "candidate" solutions are obtained and one of them

$$X = [-2.486, -0.529, -0.194, 1.616, 3.455]^T \quad (5)$$

is proposed as the best LS solution according to a number of statistical criteria. Now if A1 is used to find a LS and then a TSL solution the result is

$$X = [-73.3, 98.4, -78.0, 90.7, -78.2]^T \quad (6)$$

which is very different from the solution given in Eqn. (5) despite the fact that their residual norms are quite close. It is also interesting that the norm of (5) is only about 4.6 compared with 188 for that of (6) and that the smallness of norm is one of the criteria mentioned above for preferring one solution to another. The TSL solution would not have found much favour from this particular viewpoint.

Example 3

This example, with

$$L = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \text{ and } M = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

is of a type often used to show that the TSL problem may not have a solution unless extra constraints are imposed [2]. Applying A1, using $X_0 = 0$, gives the LS solution $[1,0]^T$, continuing until convergence now gives the TSL solution $[1.61803,0]^T$. Another much used method for solving problems of the kind considered in this paper involves some form of direct minimization (see, e.g., [8]) as in the following treatment.

Let

$$\begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \end{pmatrix}, \begin{pmatrix} x_5 \\ x_6 \end{pmatrix} \text{ and } \begin{pmatrix} x_7 \\ x_8 \end{pmatrix}$$

be estimates of L, X and M respectively; form

$$f_1 = (1 - x_1)^2 + x_2^2 + x_3^2 + x_4^2 + (1 - x_1 x_5 - x_2 x_6)^2 + (1 - x_3 x_5 - x_4 x_6)^2 .$$

or alternatively, with more variables involved,

$$f_2 = (1 - x_1)^2 + x_2^2 + x_3^2 + x_4^2 + (1 - x_7)^2 + (1 - x_8)^2 + (x_7 - x_1 x_5 - x_2 x_6)^2 + (x_8 - x_3 x_5 - x_4 x_6)^2 \quad (8)$$

and minimize f_1 or f_2 with respect to all of the variables involved in each case. So, for example, using "Find Minimum" from "MATHEMATICA" on f_1 the solution

$$X = [x_5, x_6]^T = [1.61803, 0]^T \quad (9)$$

is obtained and using f_2 gives the solution

$$X = [x_5, x_6]^T = [1.41421, 0]^T \quad (10)$$

Notice that the solution given in Eqn.(9) is the same as that found by A1. The similar, but simpler example with $L = [a, b]^T$ and $M = [1,1]^T$ can be analysed algebraically to quantize the difference between using

f_1 and f_2. Thus, for example, taking $L = [1, -0.95]^T$ gives solutions $X = 2.37165$ and $X = 0.0553169$ using f_1 and f_2 respectively. (Again using f_1 gives the same solution as A1 and as the SVD formula given in Example 1.)

Example 4

This is similar to Example 3 but rather more sophisticated; it is taken from [2] where it is analysed using SVD,

$$L = \begin{bmatrix} \sqrt{6} & \sqrt{6} \\ \sqrt{2}/4 & -\sqrt{2}/4 \\ \sqrt{2}/2 & \sqrt{2}/2 \end{bmatrix}, \qquad M = \begin{bmatrix} 2 \\ 0 \\ -\sqrt{3} \end{bmatrix}.$$

Using $X_0 = 0$ as the starting approximation in A1 gives the LS solution

$$X_{LS} = [0.282633, 0.282633]^T$$

and then proceeding to convergence gives the TLS solution

$$X_{TLS} = [0.408248, 0.408248]^T$$

Notice that this is the same as the solution $[1/\sqrt{6}, 1/\sqrt{6}]^T$ given in [2].

In the same manner, as for the previous example, setting up the appropriate f_1 and using FindMinimum gives

$$X = [0.408245, 0.408425]^T$$

and with the appropriate f_2 the solution

$$X = [0.34186, 0.34186]^T,$$

is obtained.

Example 5

The final example is concerned with parameter fitting and is taken from [8]. Here

$$L = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0.9 & 1.8 & 2.6 & 3.3 & 4.4 & 5.2 & 6.1 & 6.5 & 7.4 \end{bmatrix}^T$$

and

$$M = [5.9, 5.4, 4.4, 4.6, 3.5, 3.7, 2.8, 2.8, 1.4, 1.5]^T$$

In this example the first column of L is fixed and so one method of proceeding is as follows. [2]; $[L;M]$ is multiplied by a suitable Householder matrix to give the new matrix

$$\begin{bmatrix} 3.16228 & 12.0799 & 11.7004 \\ 0 & -4.68666 & 2.71745 \\ 0 & -3.78666 & 1.71745 \\ 0 & -2.98666 & 1.91745 \\ 0 & -2.28666 & 0.817446 \\ 0 & -1.18666 & 1.01745 \\ 0 & -0.386656 & 0.117446 \\ 0 & 0.513344 & 0.117446 \\ 0 & 0.913344 & -0.282554 \\ 0 & 1.81334 & -1.18255 \end{bmatrix}$$

and algorithm A1 is now applied to the submatrix obtained by deleting the first row and column of the above matrix to give the second component x_2 of the solution vector X. The first component x_1 of X is then obtained from

$$3.16228\, x_1 = 11.7004 - 12.0799 x_2 \; ;$$

in this way

$$X = [5.78403, -0.545562]^T$$

is obtained.

Direct minimization can also be used as in the two previous examples to give the two solutions

$$X = [5.78404, -0.545561]^T$$

and

$$X = [5.82535, -0.551802]^T$$

using sums of squares similar to f_1 and f_2 respectively.

Conclusion

It has been demonstrated that an algorithm for solving the AMRE can be used to solve over-determined systems of linear equation. A number of numerical examples illustrate the techniques involved.

SYMBOLS

F, G, L, M, P, Q, V, W	Coefficients in algebraic matrix Ricatti equation (AMRE).
X	Solution of AMRE.
X_i	iterates in solution to AMRE
$[A;B]$	concatenated matrix formed from matrices A and B
$A, B, C, R, S, \alpha, \beta, M, T$	matrices defined in Appendix
A^T	transpose of matrix A
A^+	pseudo-inverse of matrix A
$A1, A2$	algorithms from [6]
SVD	singular value decomposition
x_i	components of vector or matrix X
LS	least squares
TLS	total least squares
i	running index

f_1, f_2 sums of squares defined in Eqns. (7) and (8)
$\|A\|_E$ Eudidian norm of A
e Eudidian norm of residual error in solution of AMRE
m, n, p integers used to give order of matrices

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APPENDIX

Algorithm A1

To solve the general AMRE

$$XPX + QX + XF + G = O$$

Let X_0 be an approximate solution. Let $i = 0$

Compute:

$$A_i = X_i P + Q$$
$$B_i = PX_i + F$$
$$C_i = X_i P X_i - G$$
$$R_i = (I_n - A_i)^{-1}$$
$$S_i = (I_n - B_i)^{-1}$$
$$\alpha_i = 2R_i - I_n$$
$$\beta_i = 2S_i - I_n$$
$$M_i = -2R_i C_i S_i$$
$$T_1^{(i)} = M_i$$
$$T_2^{(i)} = T_1^{(i)} + \alpha_i T_1^{(i)} \beta_i$$
$$T_3^{(i)} = T_2^{(i)} + \alpha_i^2 T_2^{(i)} \beta_i^2$$

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$$T_{k+1}^{(i)} = T_k^{(i)} + \alpha_i^{2^{(k-1)}} T_k^{(i)} \beta_i^{2^{(k-1)}}$$

When converged set $X_{i+1} = T_{k+1}^{(i)}$, $i = i + 1$
REPEAT