ON BEST APPROXIMATE SOLUTIONS OF LINEAR MATRIX EQUATIONS

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Communicated by J. A. Todd

Received 15 February 1955

In an earlier paper (4)‡ it was shown how to define for any matrix a unique generalization of the inverse of a non-singular matrix. The purpose of the present note is to give a further application which has relevance to the statistical problem of finding 'best' approximate solutions of inconsistent systems of equations by the method of least squares. Some suggestions for computing this generalized inverse are also given.

Notation. In this paper capital letters always denote matrices (square or rectangular) with real or complex elements, the conjugate transpose of the matrix A (or simply the transpose if A is real) being written A^*. The shapes of matrices occurring in expressions are assumed unrestricted except by considerations of conformability. The symbol I denotes any suitable unit matrix.

The generalized inverse of A is defined (as in (4)) to be the unique matrix $A^\dagger$ satisfying

$$AA^\dagger A = A, \quad A^\dagger AA^\dagger = A^\dagger, \quad (AA^\dagger)^* = AA^\dagger, \quad (A^\dagger A)^* = A^\dagger A.$$

If A is real, so also is $A^\dagger$, since it is unique; if A is non-singular, then $A^\dagger = A^{-1}$.

I shall make use of the following relations, all of which are to be found in (4), but which are also immediate consequences of the above:

$$A^*AA^\dagger = A^*, \tag{1}$$

$$A^{\dagger\dagger} = A, \tag{2}$$

$$A^\dagger AA^\dagger = A^\dagger, \tag{3}$$

$$A^*A^{\dagger *}A^\dagger = A^\dagger. \tag{4}$$

I use the notation $\| A \|$ for the sum of the squares of the moduli of the elements of A. Clearly $\| A \| = \operatorname{trace} A^*A$, and $\| A \| > 0$ unless $A = 0$.

Definition. I shall say that X_0 is a *best approximate solution* of the equation $f(X) = G$ if for all X, either

$$\text{(i)} \quad \| f(X) - G \| > \| f(X_0) - G \|,$$

or

$$\text{(ii)} \quad \| f(X) - G \| = \| f(X_0) - G \| \quad \text{and} \quad \| X \| \geqslant \| X_0 \|.$$

Theorem. *$A^\dagger B$ is the unique best approximate solution of the equation $AX = B$.*

Proof. We have the identity

$$\| AP + (I - AA^\dagger) Q \| = \| AP \| + \| (I - AA^\dagger) Q \|, \tag{5}$$

‡ See also Moore (3) and a forthcoming note by R. Rado.

since (1) implies

$$\{AP+(I-AA^{\dagger})Q\}^*\{AP+(I-AA^{\dagger})Q\} = (AP)^*AP+\{(I-AA^{\dagger})Q\}^*(I-AA^{\dagger})Q.$$

Thus, in particular,

$$\begin{aligned}\|AX-B\| &= \|A(X-A^{\dagger}B)+(I-AA^{\dagger})(-B)\| \\ &= \|AX-AA^{\dagger}B\|+\|AA^{\dagger}B-B\| \geqslant \|A(A^{\dagger}B)-B\|,\end{aligned}$$

with equality only when $AX = AA^{\dagger}B$. Replacing A by $A^{\dagger}$ in (5) and using (2), we deduce $\|A^{\dagger}B+(I-A^{\dagger}A)X\| = \|A^{\dagger}B\|+\|(I-A^{\dagger}A)X\|$. Thus, if $AX = AA^{\dagger}B$, (3) gives $\|X\| = \|A^{\dagger}B\|+\|X-A^{\dagger}B\|$, from which the theorem follows.

COROLLARY 1. *The general linear matrix equation* $A_{(1)}XC_{(1)}+\ldots+A_{(m)}XC_{(m)} = B$ *has a unique best approximate solution.*

Proof. This equation is only apparently more general than that of the theorem, since it can be written as

$$\sum_{\beta,\gamma}\left(\sum_{r=1}^{m} a_{(r)\alpha\beta}\,c_{(r)\gamma\delta}\right)x_{\beta\gamma} = b_{\alpha\delta},$$

where $A_{(r)} = (a_{(r)\alpha\beta})$, etc. This is of the form $RX = S$, where X and S are vectors.

In particular, the equation $AXC = B$ can be treated in this way, the best approximate solution being $A^{\dagger}BC^{\dagger}$. This result can also be obtained from the identity

$$\|APC+Q-AA^{\dagger}QC^{\dagger}C\| = \|APC\|+\|Q-AA^{\dagger}QC^{\dagger}C\|.$$

COROLLARY 2. *The best approximate solution of* $AX = I$ *is* $A^{\dagger}$.

This shows that $A^{\dagger}$ is the only matrix having all those properties required of it for the theorem and suggests a possible alternative definition of $A^{\dagger}$.

The equation $AX = B$, where X and B are vectors, is of special interest in statistics, its best approximate solution being that required in the method of least squares when the equation has no actual solution (see (5)). It would appear, therefore, that a suitable method of computing $A^{\dagger}$ from the matrix A might be of value. In most practical cases, however, the matrix A^*A is non-singular, so that $A^{\dagger} = (A^*A)^{-1}A^*$. This gives nothing different from the conventional method of solution (see also (1)).

It is possible to calculate $A^{\dagger}$ even when A^*A and AA^* are both singular by either of the following methods.

Method 1. Any matrix can be partitioned in the form

$$\begin{pmatrix} A & B \\ C & CA^{-1}B \end{pmatrix}$$

(using a suitable arrangement of rows and columns), A being any non-singular submatrix whose rank is equal to that of the whole matrix. It is then easily verified that

$$\begin{pmatrix} A & B \\ C & CA^{-1}B \end{pmatrix}^{\dagger} = \begin{pmatrix} A^*PA^* & A^*PC^* \\ B^*PA^* & B^*PC^* \end{pmatrix},$$

where $P = (AA^*+BB^*)^{-1}A(A^*A+C^*C)^{-1}$. The matrices AA^*+BB^* and A^*A+C^*C are positive definite, since A is non-singular. Thus the generalized inverse of any matrix can be expressed in terms of ordinary reciprocals of matrices.

Method 2. The generalized inverse of a given matrix A can be obtained from any matrix D satisfying $A^*A = D(A^*A)^2$, since multiplication on the right by $A^\dagger A^{\dagger *} A^\dagger$ gives $A^\dagger = DA^*$ (from (1) and (4)). Now put $B = A^*A = (b_{\alpha\beta})$, and define a sequence of matrices $C_{(j)}$ for $j = 1, 2, \ldots$ by

$$\left.\begin{aligned} C_{(1)} &= I, \\ C_{(j+1)} &= I \,.\, \frac{1}{j}\,\mathrm{trace}\,(C_{(j)}B) - C_{(j)}B \quad (j = 1, 2, \ldots). \end{aligned}\right\} \tag{6}$$

I shall show that $C_{(r+1)}B = 0$ and $\mathrm{trace}\,(C_{(r)}B) \neq 0$, where r is the rank of B, so that if $D = \dfrac{rC_{(r)}}{\mathrm{trace}\,(C_{(r)}B)}$, then $DB^2 = B$ as required.

$$\text{Let}\quad c_{(1)\alpha\beta} = \delta_{\alpha\beta}, \quad c_{(j+1)\alpha\beta} = \frac{1}{j!}\sum_{\gamma_1, \ldots, \gamma_j} \begin{vmatrix} b_{\gamma_1\gamma_1} & \cdots & b_{\gamma_1\gamma_j} & \delta_{\gamma_1\beta} \\ \vdots & & \vdots & \vdots \\ b_{\gamma_j\gamma_1} & \cdots & b_{\gamma_j\gamma_j} & \delta_{\gamma_j\beta} \\ b_{\alpha\gamma_1} & \cdots & b_{\alpha\gamma_j} & \delta_{\alpha\beta} \end{vmatrix} \quad (j = 1, 2, \ldots).$$

The summation extends over all the ordered sets $\gamma_1, \ldots, \gamma_j$; so that each non-zero term of the sum is repeated $j!$ times. Expanding by Laplace's rule with respect to the last column, we get

$$c_{(j+1)\alpha\beta} = \delta_{\alpha\beta}\frac{1}{j!}\sum_{\gamma_1, \ldots, \gamma_j} \begin{vmatrix} b_{\gamma_1\gamma_1} & \cdots & b_{\gamma_1\gamma_j} \\ \vdots & & \vdots \\ b_{\gamma_j\gamma_1} & \cdots & b_{\gamma_j\gamma_j} \end{vmatrix} - j\,\frac{1}{j!}\sum_{\gamma_1, \ldots, \gamma_{j-1}} \begin{vmatrix} b_{\gamma_1\gamma_1} & \cdots & b_{\gamma_1\gamma_{j-1}} & b_{\gamma_1\beta} \\ \vdots & & \vdots & \vdots \\ b_{\gamma_{j-1}\gamma_1} & \cdots & b_{\gamma_{j-1}\gamma_{j-1}} & b_{\gamma_{j-1}\beta} \\ b_{\alpha\gamma_1} & \cdots & b_{\alpha\gamma_{j-1}} & b_{\alpha\beta} \end{vmatrix}.$$

Comparing this with (6) we see that $C_{(j)} = (c_{(j)\alpha\beta})$. Now if B is of rank r, $C_{(r+1)}B$ is zero, since its elements are sums of minors of B of order $r+1$. Also, $\mathrm{trace}\, C_{(r)}B$ is not zero, since it is r times the sum of the principal minors of B of order r, and B is a positive semi-definite matrix.

Thus, relation (6) affords a repetitive method of computing $A^\dagger$, while the definition of $c_{(j)}$ leads to an explicit form for $A^\dagger$ when the rank of A^*A (i.e. of A) is known.

If the matrix B is replaced by any non-singular matrix, the above argument still holds, giving $D = B^{-1}$. This is essentially Frame's method of computing the inverse of a matrix (see (2)).

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