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A SPECIAL FORM OF A GENERALIZED INVERSE OF AN ARBITRARY COMPLEX MATRIX

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SUMMARY

The primary concern of this paper is to investigate the problem of inversion of singular or nonsquare matrices. In this connection, a new algorithm for computing the generalized inverse of an arbitrary complex matrix is given. For a nonsingular matrix the algorithm gives the ordinary inverse of the matrix.

The paper is divided into several sections. The first two sections give a definition-theorem exposé of the known results in the literature. The following sections give a new explicit form, together with an algorithm for computing the new explicit form. An application to least squares approximation is given that can easily be realized in trajectory analysis problems. Finally, a computer program for computing the generalized inverse of a matrix is given utilizing the algorithm mentioned in the latter paragraph.

INTRODUCTION

A. Bjerhammar (ref. 1), E. H. Moore (ref. 2), and R. Penrose (ref. 3) independently generalized the concept of matrix inversion to include arbitrary complex matrices. Their equivalent forms of the generalized inverse of a matrix have given rise to many applications of generalized inversion. In the text, the basic theory is utilized in giving a new explicit form of the generalized inverse of an arbitrary complex matrix.

SYMBOLS

Capital letters	matrices unless otherwise stated
Lowercase letters	column vectors unless otherwise stated or clear from context
A^*	matrix conjugate transpose of A
A^{-1}	matrix inverse for nonsingular A

A^+	generalized inverse of A
H	a Hermitian idempotent matrix (h.i.); that is, a matrix such that $H^* = H$ and $HH = H$
$R(A)$	range space of A; that is, the collection of all images of column vectors under the transformation A
$P_{R(A)}$	orthogonal projection on the range of A; that is, a Hermitian idempotent leaving R(A) fixed
E^m	m-dimensional euclidean space
$\mathrm{diag}(a_1, a_2, \ldots, a_n)$	diagonal matrix

DEFINITIONS AND EQUIVALENT FORMS

A. Bjerhammar (ref. 1), E. H. Moore (ref. 2), and R. Penrose (ref. 3) independently generalized the concept of matrix inversion to include arbitrary complex matrices. The generalized inverse of a singular, or nonsquare, matrix possesses properties which make it a central concept in matrix theory.

In this paper, a definition-theorem expose is presented, along with applicable references and special problems. The following fundamental theorem due to Penrose (ref. 3) is stated without proof:

THEOREM I. The four equations

$$AXA = A \tag{1}$$

$$XAX = X \tag{2}$$

$$(AX)^* = AX \tag{3}$$

$$(XA)^* = XA \tag{4}$$

have a unique solution X for each complex matrix A.

Definition 1. The solution X in THEOREM 1 is denoted $X = A^+$ and is called the generalized inverse of A.

The following theorem gives an equivalent form of A^+.

THEOREM II. For any $m \times m$ matrix A over the complex field, $X = A^+$ is the unique solution to the equations $AX = P_{R(A)}$ and $XA = P_{R(X)}$

where $R(A)$ is the range space of A in E^m and $P_{R(A)}$ is the orthogonal projection on $R(A)$.

Proof: THEOREM I implies that AX is a Hermitian idempotent (see Symbols) which leaves A fixed, that is, $(AX)A = A$. Hence, AX must be a projection. It may be concluded that XA is also a projection.

The properties of the generalized inverse and possible computing schemes are given in the following theorem.

THEOREM III. Let A be an arbitrary complex matrix. Then, for scalar $\lambda \neq 0$ and unitary U and V,

$$A^+(A^+)^*A^* = A^+ = A^*(A^+)^*A^+ \tag{5}$$

$$A^+AA^* = A^* = A^*AA^+ \tag{6}$$

$$(A^+)^+ = A \tag{7}$$

$$(A^*)^+ = (A^+)^* \tag{8}$$

$$A^+ = A^{-1} \quad \text{for nonsingular } A \tag{9}$$

$$(\lambda A)^+ = \frac{1}{\lambda}A^+ \tag{10}$$

$$(A^*A)^+ = A^+(A^+)^* \tag{11}$$

$$(UAV)^+ = V^{-1}A^+U^{-1} \tag{12}$$

$$\left.\begin{array}{l} A = \sum A_i \quad \text{and} \quad A_i^*A_j = 0 \\ A_j^*A_i = 0 \quad \text{for} \quad i \neq j \\ \text{imply} \quad A^+ = \sum A_i^+ \end{array}\right\} \tag{13}$$

If A is normal (i.e., $A^*A = AA^*$) then

$$A^+A = AA^+ \quad \text{and} \quad (A^n)^+ = (A^+)^n \tag{14}$$

A, A^*A, A^+, and A^+A all have rank equal to trace (A^+A) (15)

$$A^+ = (A^*A)^+A^* \tag{16}$$

Equation (16) reduces the problem of computing A^+ to that of computing the generalized inverse of a Hermitian matrix A^*A. Moreover, such a matrix can always be diagonalized by a unitary transformation, that is,

$$D = U(A^*A)V = \mathrm{diag}\left(a_1, \ldots, a_n\right)$$

Equations (10) and (12) imply that

$$(A^*A)^+ = VD^+U = V\,\mathrm{diag}\left(\frac{1}{a_1}, \ldots, \frac{1}{a_n}\right)U$$

It is tacitly assumed that if $a_i = 0$, the corresponding term in $\mathrm{diag}\left(\frac{1}{a_1}, \ldots, \frac{1}{a_n}\right)$ is zero. It is not usually an easy task to determine the unitary transformations U and V. Methods for computing the generalized inverse have been given by various authors (refs. 1, 4, 5, 6, and 7).

The following is a theorem of major importance characterizing all solutions of the matrix equations $AXB = C$ which have some solution X.

<u>THEOREM IV</u>. For the matrix equation $AXB = C$ to have a solution, a necessary and sufficient condition is

$$AA^+CB^+B = C$$

in which case, the general solution is

$$X = A^+CB^+ + Y - A^+AYBB^+$$

where Y is arbitrary to within the limits of being consistent with the dimension in the indicated multiplications (ref. 3).

Proof: If X satisfies $AXB = C$,

$$C = AXB = AA^+AXBB^+B = AA^+CB^+B$$

Conversely, if $C = AA^+CB^+B$, A^+CB^+ is a particular solution. Clearly, for the general solution, $AXB = 0$ must be solved. Any expression of the form

$$X = Y - A^+AYBB^+$$

The only property required of A^+ and B^+ in the theorem is $AA^+A = A$ and $BB^+B = B$.

Corollary A. The general solution to the vector equation

$$Px = c$$

is

$$x = P^+c + (I - P^+P)y$$

where y is arbitrary, provided a solution exists.

Corollary B. A necessary and sufficient condition for the equations

$$AX = C$$

and

$$XB = D$$

to have a common solution is that each have a solution and $AD = CB$ (ref. 8).

Proof: If $AX = C$ and $XB = D$ have a common solution, then clearly each has a solution and

$$AXB = CB$$

$$AXB = AD$$

so that

$$CB = AD$$

In order to obtain the sufficiency of the condition, it is assumed that

$$X = A^+C + DB^+ - A^+ADB^+$$

which is a solution if $AD = CB$, $AA^+C = C$, and $DB^+B = D$.

THEOREM V.

$$A^+A,\ AA^+,\ I - A^+A, \text{ and } I - AA^+ \text{ are h.i.} \tag{17}$$

$$H \text{ is h.i. implies } H^+ = H \tag{18}$$

(See Symbols.)

Proof: The proof requires a straightforward application of THEOREM I.

In general, the reversal rule (i.e., $(AB)^+ = B^+A^+$ as in the case of the standard inverse) does not hold. R. Cline (ref. 9) recently obtained the following result:

THEOREM VI. Let A and B be matrices with the product AB defined. Then,

$$(AB)^+ = B_1^+A_1^+$$

where:

$$AB = A_1B_1$$

$$B_1 = A^+AB$$

and

$$A_1 = AB_1B_1^+$$

THE EXPLICIT FORM

Utilizing the properties of A^+ in the preceding sections, an explicit form is developed which gives rise to an algorithm for computing the generalized inverse of an arbitrary complex matrix (ref. 5).

THEOREM VII. For any matrix A, $A^+ = WAY$ where W and Y are any solutions of

$$WAA^* = A^* \tag{19}$$

and

$$A^*AY = A^* \tag{20}$$

Proof: Equations (19) and (20) indeed have a solution $W = Y = A^+$. Moreover, if W and Y are any solutions,

$$AWAA^* = AA^* \text{ and } A^*AYA = A^*A$$

so that

$$AWA = A \quad \text{and} \quad AYA = A$$

Note: $BAA^* = CAA^*$ implies $BA = CA$

In addition,

$$WAA^*W^* = A^*W^* \quad \text{and} \quad Y^*A^*AY = Y^*A^*$$

imply

$$(WA)^* = WA \quad \text{and} \quad (AY)^* = AY$$

If it is assumed that $X = WAY$, X satisfies equations (1) to (4) of THEOREM I so that $A^+ = X = WAY$.

Corollary C. For any matrix A, $A^+ = A^*S_1AS_2A^*$ where S_1 and S_2 are, respectively, any solutions of

$$(AA^*)S_1(AA^*) = (AA^*)$$

and

$$(A^*A)S_2(A^*A) = (A^*A)$$

Proof: According to THEOREM III, $W = A^*S_1$ and $Y = S_2A^*$ are solutions of equations (19) and (20) of THEOREM VII provided

$$(AA^*)S_1(AA^*) = (AA^*)$$

and

$$(A^*A)S_2(A^*A) = (A^*A)$$

The corollary follows.

<u>THEOREM VIII</u>. If B is a matrix and nonsingular matrices P and Q exist so that $PBQ = E$ is an idempotent, then $\bar{B} = QEP$ is a solution of $BXB = B$.

Proof: If P, Q, and E satisfy the hypothesis of the theorem,

$$B = P^{-1}EQ^{-1}$$

and

$$B\bar{B}B = \left(P^{-1}EQ^{-1}\right)QEP\left(P^{-1}EQ^{-1}\right) = P^{-1}EQ^{-1} = B$$

Corollary C and THEOREM VIII suggest an algorithm for computing the generalized inverse of a complex matrix F. Consider the equation $F^+ = (F^*F)^+F^*$ from reference 10, which reduces the problem of finding F^+

to that of finding the generalized inverse of the Hermitian matrix $F^*F = C$. Since $\left(C^2\right)^* = C^2$, nonsingular matrices P and Q exist (products of elementary matrices obtained by simple elimination) so that

$$PC^2Q = \begin{pmatrix} I_r & Z \\ Z & Z \end{pmatrix} = I_o$$

where I_r is a rank r identity matrix and the Z is a zero matrix. When C is set equal to A in Corollary C,

$$A^*A = AA^* = C^*C = CC^* = C^2$$

According to THEOREM VIII, solutions $S_1 = S_2 = QI_oP$ are chosen so that

$$C^+ = (CS_1)^2C$$

$$(F^*F)^+ = C^+$$

and finally,

$$F^+ = C^+F^*$$

Computing programs for calculating S_1 and S_2 are now in existence (e.g., STORM, Statistically Oriented Matrix Program, IBM). In general, these programs only compute some solution of the equation $AXA = A$, usually different from A^+. These results allow one to construct a solution to all four Penrose equations (eqs. (1) to (4) of THEOREM I), given only a solution of the first, namely, $AXA = A$.

APPLICATION TO LEAST SQUARES APPROXIMATION

In this section, an application to the least squares approximation is stated that can be realized in trajectory analysis problems. For the sake of simplicity, weighting is not considered; however, it would introduce no difficulty.

The vector equation $Ax = b$ does not, in general, have a solution x. However, all candidates for a least squares solution (i.e., a solution vector x minimizing $(Ax - b)^*(Ax - b)$) must be solutions of the normal equations (ref. 6).

$$A^*Ax = A^*b$$

THEOREM IX. Let A be any matrix $(m \times n)$ and b be any vector $(m \times 1)$. The equation

$$A^{*}Ax = A^{*}b$$

always has a solution, and hence a general solution is given by

$$x = (A^{*}A)^{+}A^{*}b + \left[I - (A^{*}A)^{+}A^{*}A\right]y$$

$$= A^{+}b + (I - A^{+}A)y$$

Moreover, if $A^{*}A$ is nonsingular, the solution is

$$x = A^{+}b$$

and is unique.

Proof: First, it is shown that

$$A^{*}Ax = A^{*}b \tag{21}$$

has a solution. Consider the vector

$$x = A^{+}b$$

Since equation (6) of THEOREM III implies $A^{*}A(A^{+}b) = A^{*}b$, $x = A^{+}b$ is indeed a solution of equation (21). The existence of this solution, together with Corollary A, implies that the general solution to equation (21) is

$$x = (A^{*}A)^{+}A^{*}b + \left[I - (A^{*}A)^{+}A^{*}A\right]y \tag{22}$$

By using equation (16) of THEOREM III,

$$x = A^{+}b + (I - A^{+}A)y$$

Finally, if $A^{*}A$ is nonsingular, then

$$x = (A^{*}A)^{+}A^{*}b + (I - I)y$$

$$= A^{+}b$$

and equation (21) has a unique solution.

In summary, if x is a least squares solution of $Ax = b$, then x must satisfy

$$A^{*}Ax = A^{*}b$$

All solutions of this equation are given by

$$x = A^+b + (I - A^+A)y$$

Any vector of the form

$$x = A^+b + (I - A^+A)y$$

is a "candidate" for a least squares solution, and this form describes the "class of all candidates."

Corollary D. Every solution of

$$A^*Ax = A^*b$$

minimizes

$$Q = (Ax - b)^*(Ax - b)$$

provided Q has a minimum.

Proof: Any vector at which Q is minimum is of the form

$$x = A^+b + (I - A^+A)y$$

If Q has a minimum, let

$$x_1 = A^+b + (I - A^+A)y_2$$

be any other solution. In order to show that

$$(Ax_1 - b)^*(Ax_1 - b) = (Ax_2 - b)^*(Ax_2 - b)$$

Ax_1 and Ax_2 is examined in light of THEOREM I.

$$\begin{aligned} Ax_1 &= A\left[A^+b + (I - A^+A)y_1\right] \\ &= AA^+b + (A - AA^+A)y_1 \\ &= AA^+b + (A - A)y_1 \\ &= AA^+b \end{aligned}$$

Similarly,

$$Ax_2 = AA^+b$$

so that

$$Ax_1 - b)^*(Ax_1 - b) = (Ax_2 - b)^*(Ax_2 - b)$$

that is, every vector of the form

$$x = A^+b + (I - A^+A)y$$

yields the same minimum value of Q.

SUBROUTINE GENINV

GENINV is a FORTRAN IV subroutine used to compute the generalized inverse of an mxn matrix A. All computations are made in double-precision floating point arithmetic. The subroutine is based on the algorithm suggested by the explicit form.

Calling Sequence

Call GENINV (A, AP, M, N, L, E)

where:

A double-dimensioned, double-precision array containing the original matrix. A is dimensioned A(25, 25)

AP double-dimensioned, double-precision array where the generalized inverse of A will be computed. AP is dimensioned AP(25, 25)

M number of rows in the original matrix

N number of columns in the original matrix

L twice N

E some small number for near-zero divisor test

Method

Given A (Print A)

Compute:

$$C = A^* A \qquad \text{(Print C)}$$

$$C^2 = CC \qquad \text{(Print } C^2\text{)}$$

Find nonsingular matrices E and P such that

$$EC^2P = \begin{pmatrix} I_r & Z \\ Z & Z \end{pmatrix} = I_o$$

(Print E, P, I_o)

(A form of Gaussian elimination with pivoting employed)

Compute:

$$R = PI_oE \qquad \text{(Print R)}$$

then

$$C^+ = CRCRC \qquad \text{(Print } C^+\text{)}$$

also

$$A^+ = C^+A^* \qquad \text{(Print } A^+\text{)}$$

Remarks

The program uses two double-precision arrays CSQ(50, 50) and B(25, 25) for internal manipulation. The subroutine leaves the original matrix A intact.

Results are printed after each step as indicated.

CONCLUSION

The theory developed in THEOREMS VII and VIII gives rise to easy calculation of the generalized inverse of an arbitrary complex matrix when only the solution to the matrix equation $AXA = A$ can be found. In general, a simultaneous solution must be found for four matrix equations, given in THEOREM I, that define the generalized inverse.

Manned Spacecraft Center
National Aeronautics and Space Administration
Houston, Texas, February 5, 1965

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