## COMPUTATION OF THE PSEUDOINVERSE OF

A MATRIX OF UNKNOWN RANK


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# COMPUTATION OF THE PSEUDOINVERSE OF 

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by

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Abstract
27058
A program is described which computes the pseudoinverse, and other related quantities, of an $m \times r$ natrix $A$ of unknown rank. The program obtains least square solutions to singular and/or inconsistent linear systems $A x=B$, where $m \leq n$ or $m>n$ and the rank of $A$ may be less than $\min (m, n)$. A complete description of the program and its use is given, including computational experience on a variety of problems.


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## I. Introduction.

A method for the computation of the pseudoinverse, and other related quantities, corresponding to an $m \times n$ matrix $A$ of unknown rank $r$, has recently been described [5]. The method determines the pseudoinverse $A^{+}$of $A$ and a related matrix $A^{\#}$. The pseudoinverse has the property that given the linear system $A x=b$, the solution $x_{m}=A^{+} b$ satisfies $\left\|A x_{m}-b\right\| \leq\|A x-b\|$ for all $x$, and $\left\|x_{m}\right\| \leq\|x\|$ for all $x$ such that $\left\|A x_{m}-b\right\|=\|A x-b\|$. The minimum basic solution $x_{b}=A^{\#} b$ has the property that $\left\|A x_{b}-b\right\| \leq\|A x-b\|$ for all $x$, and $x_{b}$ has at most $r$ non-zero elements.

The computational difficulty for this problem arises primarily because the rank $r$ is not known. In particular, it may be difficult to assign the correct rank if one or more of the singular values of $A$ are small but non-zero [3]. Several other recent papers [1], [2], [4], on the computation of the pseudoinverse have not considered this important practical question.

The approach used here to handle this difficulty can be summarized as follows. The desired matrices $A^{\#}$ and $A^{+}$are formed from a matrix B, which consists of linearly independent columns selected from A.

We would like to determine $B$ so that it spans the same space as $A$, in which case $B$ will contain $r$ columns. Suppose we have a matrix $B_{q}$ with $q$ linearly independent columns selected from $A$, (where $q<r$ ) and the corresponding approximation $A_{q}^{+}$to $A^{+}$. Adding another linearly independent column of $A$ to $B_{q}$, giving $B_{q+1}$, should give an improved approximation $A_{q+1}^{+}$to the pseudoinverse. However, due to roundoff error in the calculation it may turn out for an ill-conditioned system that the new approximation is actually worse in the sense that $\left\|A A_{q+1}^{+}-I\right\|>\left\|A A_{q}^{+}-I\right\|$. Such a test is made in the pseudoinverse determination with the result that the effective rank of $A$ (the number of columns in $B$ ) is the maximum possible consistent with minimizing the error $\| \mathrm{AA}^{+}$- I\|.

A closely related aspect of the method used here to compute the pseudoinverse is what might be called its "smoothing" property. In many practical situations one would like to obtain a solution to a linear system which is stable in the sense that small changes in the matrix elements do not cause large changes in the solution vector. In general, the solution $x=A^{+} b$, where $A^{+}$is the true pseudoinverse, will not behave smoothly. In fact, the norm of x will increase without bound as a singular value of $A$ approaches zero. This difficulty can be eliminated by imposing a predetermined upper bound on the norm of $\left(B^{\prime} B\right)^{-1}$. This is accomplished by estimating the effect of adding a new column of A to $B_{q}$ and only adding this new column to $B_{q}$ if it does not cause any element of $A_{q+1}^{+}$to exceed the bound. Details of this selection procedure and the manner in which it depends on the choice of the bound SUPER is discussed in the next section.

In Section 3 the use of the Algol program, written to perform this algorithm, is described and suggested values for the input parameters are given. The program use is illustrated by means of a sample problem. A large number of problems have been solved using this program. Several different kinds of tests have been performed:
a) Very ill-conditioned matrices like the segments of the Hilbert matrix [6] have given a clear example of the smoothing property of the method.
b) Random rectangular matrices of random sizes have been generated and the pseudoinverse have been computed. The sizes were allowed to vary between 1 and 25. In all the cases the results were satisfactory. c) Same as in b) but with random ranks. In every case the rank was correctly determined by the program.
d) Random matrices of specified size covering a range of values of $\underline{m}$ and $n$ were run in order to obtain time estimates for different size problems.
e) A number of least-square problems, i.e., with $m \gg n$ and only one right-hand side.
f) A variety of matrices for which an independent check on the accuracy of the solution was available.

Tests b) through f) showed that in reasonable problems in which the rank is well determined the program will work very well, while a) has shown that in very ill-conditioned cases the smoothing property of the method is effective.

These test results are discussed more fully in Section 4. The notation used in [5] will also be followed here.

Details of storage requirements are given in Section 5 .
A copy of the program appears in the Appendix.

## II. Program Description.

The method used to compute $A^{\#}$ and $A^{+}$from $B$ is essentially that given in Section 2 of [5]. For convenience we will repeat the key relations here. The pseudoinverse of the $m \times r$ matrix $B$ of rank $r$ is given by

$$
\begin{equation*}
B^{+}=\left(B^{\prime} B\right)^{-1} B^{\prime} \tag{2.1}
\end{equation*}
$$

The non-zero rows of the $n x m$ matrix $A^{\#}$ then consists of the corresponding rows of $B^{+}$. An $r x n$ matrix of rank $r$ is also obtained from $\mathrm{B}^{+}$according to

$$
\begin{equation*}
C=B^{+} A \tag{2.2}
\end{equation*}
$$

Note that, if $B$ contains all the independent columns of $A$, then $A=B C$. Finally, $A^{+}$is obtained from $C$ and $B^{+}$by

$$
\begin{equation*}
A^{+}=C^{\prime}\left(C C^{\prime}\right)^{-1} B^{+} \tag{2.3}
\end{equation*}
$$

The determination of $B$ is based on the algorithm of Section 3 in [5], using the more sophisticated selection procedure described below.

The program consists essentially of two parts. One part has all the input-output and the other is a PROCEDURE called PSEUDOINVER which may also be used separately as a part of other programs. The program solves the matricial problem,

$$
\begin{equation*}
A X=R H S \tag{2.4}
\end{equation*}
$$

where RHS is a matrix containing several right hand sides.
a) The first part of PSEUDOINVER normalizes the matrix $A$ by scaling each column so that its Euclidean norm is equal to one. The normalization constants are saved in order to get back to the original problem.

The search for independent columns of $A$ is then made to determine the matrix $B$, according to the formulas described in section 3 of [5]. At this stage, the condition for a vector to be accepted as independent of the ones already included in the basis is that $\alpha$, the square of the norm of the projection on the orthogonal subspace to that basis, be less than a quantity ORTP, which is an input parameter. Later we will discuss the appropriate choice of ORTP and the other parameters appearing in the program.

As the columns chosen in this fashion might not necessarily be the first columns of $A$, a record is kept of the column number of the accepted vectors.

After all the columns have been inspected two situations can arise; either all the $n$ columns of $A$ have been accepted or some have been rejected. In the first case we have finished and the computations indicated at the beginning of this section are performed to get $A^{+}, A \#, X_{b}$ and $X_{m}$. Other computed quantities are the residuals, $\quad N X M=\left\|A X_{m}-R H S\right\|$ $N X B=\left\|A X_{b}-R H S\right\|$ corresponding to $X_{m}$ and $X_{b}$, and $E S T=\|B C-A\|$.

EST would be zero if the computation were performed exactly; in general EST will be very small for well-conditioned matrices and will increase with the ill-conditioning or if an almost dependent column is added to $B$.

If only $q<n$ columns of $A$ are selected for inclusion in $B$ then the basis thus constructed is called $B_{q}$ and the second part of PSEUDOINVER is called.
b) The projections on the subspace orthogonal to $B_{q}$ are computed for all the rejected columns. The Euclidean norm of each projection is computed,

$$
\begin{equation*}
\alpha_{j}=\left\|\left(I-B_{q} B_{q}^{+}\right) a_{j}\right\|^{2} \tag{2.5}
\end{equation*}
$$

and the column corresponding to the maximum $\alpha_{j}$ (the most independent one) is stored in SAV.
c) A test is now performed which is based upon an estimation of the norm that $\left(B_{q+1}^{\prime} B_{q+1}\right)^{-1}$ would have if we were to include $S A V$ in the basis. The norm used is $\|A\|=\max _{i} \sum_{j=1}^{n}\left|a_{i j}\right|$ and the estimate is derived from the formula,

$$
\left(B_{q+1}^{\prime} B_{q+1}\right)^{-1}=\left(\begin{array}{c|c}
\left(B_{q}^{\prime} B_{q}\right)^{-1} & 0  \tag{2.6}\\
\hline 0 & 0
\end{array}\right)+\alpha_{q+1}^{-1}\binom{u_{q}}{-1}\left(u_{q}^{\prime} \mid-1\right)
$$

where $u_{q}=B_{q}^{+}$SAV and $\alpha_{q+1}$ is the square of the norm of the projection of SAV on the orthogonal subspace to that spanned by $B_{q}$. Then
$\left\|\left(B^{\prime}{ }_{q+1} B_{q+1}\right)\right\| \leq \operatorname{ESTIM}=\left\|\left(B_{q}^{\prime} B_{q}\right)^{-1}\right\|+\alpha_{q+1}^{-1}(1+\sqrt{q})$

If ESTIM is larger than SUPER (an input parameter) then SAV is rejected and $B_{q}$ is taken as the final $B$.

This test avoids large elements in the pseudoinverse and gives the smoothing property discussed in the introduction.
d) If the test in c) is passed then the PROCEDURE GARBG, which computes all the matrices and quantities mentioned at the beginning of this section, is called and a second test is made. GARBG is used again, now with the basis $B_{q}$ plus the column SAV. The test consists in comparing the values of $\left\|A X_{m}-R H S\right\|,\left\|A X_{b}-R H S\right\|$ and $\|B C-A\|$ obtained with one basis, with the corresponding ones obtained with the incremented basis. If all these values for $B_{q+1}$ are smaller than for $B_{q}$ then $S A V$ is definitely
accepted. After shifting all the useful quantities, part (b) is repeated for the new basis $B_{q+1}$ and so on, until either an exit is provided for one of the tests or the columns of $A$ are exhausted. All the scalar products are performed in double precision. The block diagram in Fig. I shows the most essential parts of the program.

It is worth noting that this strategy has been dictated by the problem itself and achieves the best numerical pseudoinverse possible using the method of [5] and taking into account the numerical roundoff error of the computer being used. This strategy takes advantage of the step by step algorithm for determining $B$, and constructs an independent basis, the degree of independence being determined by the parameter ORTP. By picking the most independent vector among the remaining ones, and checking to see if this decreases the residuals (by taking this vector in the basis) we are answering in a direct manner the two questions: how many columns of $A$ do we need to minimize the residual? and, among all the possible sets of independent columns, which set gives the best representation of the pseudoinverse?

Fig. 1 - BLOCK DIAGRAM

III. Program Use.

As described in the previous section, several parameters are needed besides the matrix A. Now we will explain the use and possibilities of these parameters.

Input.
M (integer) number of rows in $A$.
N (integer) number of columns in A .
$T$ (integer) number of right-hand sides.
OPC (Boolean) If OPC is equal to 1 then the program will compute the matrices $A^{+}$and $A^{\#}$, and the right-hand side RHS $=I(m \times m)$ will be automatically provided.

Moreover, OPC decides if in the test described in Section 2,d) the quality of the representation ( $A=B C$ ) is controlled. That test is done only if OPC = TRUE . If OPC is equal to FALSE then RHS an $M \times T$ matrix has to be provided and the program will compute $X_{B}=A^{\#}$.RHS, and $X_{M}=A^{+}$. RHS, matrices that will be printed out instead of $A^{+}$ and $A^{\#}$.

SUPER (real) It is the SUPER of Section 2, c). If an upper bound for the elements of $A^{+}$is known then SUPER can be set to this bound to take advantage of the smoothing property of this method; otherwise it is suggested that $10^{14}$ be used. It should be noted that, in general, a larger value than $10^{14}$
will increase computing time by throwing unnecessary decisions into the test of Section 2,d). On the other hand, much smaller values may completely eliminate from further consideration some columns which could be used to decrease the error.

ORTP (real) This parameter was described in Section 2, a). Small values for ORTP (around $10^{-4}$ ) in general will accelerate the process because the first part (construction of a basis of strongly independent column) is the fastest and as many columns as possible should be accepted there. Nevertheless, there are at least two cases in which a more careful choice of ORTP may be important. If higher precision in the answers is desired (at the cost of increased computing time), then a larger value of ORTP should be used, say 0.05. This will allow the second part of the program to choose "better" columns.

The other delicate case occurs when the matrix is very ill-conditioned and the rank is therefore not well defined. Here the use of a relatively large ORTP is important. Again values around $0: 05$ are recommended.

Summarizing, in a reasonable, well behaved problem a recommended set of parameters is:

$$
\operatorname{SUPER}=10^{14}, \quad \text { ORTP }=10^{-4} .
$$

If the representation becomes very bad (\|A-BC\| too large), the problem is not well behaved and more burden should be passed on to the second and safer test by increasing SUPER and decreasing ORTP .

If the user has information that certain variables are more significant than others, this information can be used by ordering the matrix A so that the columns of $A$ corresponding to these variables appear first. This will insure that these columns are considered first for inclusion in the basis $B$.

If the complete program is used, then only the numerical data have to be punched. This is done in the following way.

As all the read statements are in the FREE FIELD form, available in the EXTENDED ALGOL for the B5000 at Stanford, no special format is necessary. Numbers can be punched in any format, needing just one space in between to separate them.
lst. card: $\quad \mathrm{M} \quad \mathrm{N} \quad \mathrm{O}$ P C SUPER ORTP $\begin{array}{lllllll}\text { for instance } & 10 & 10 & 10 & 1 & 0.001\end{array}$

Next cards will contain the matrix A punched by rows. As each READ asks for a whole row, care must be taken not to mix different rows in the same card.

Finally, if 0 P C $=0$ the right-hand sides (RHS) have to be provided and are read by columns. Each new column must be started on a new card, so that there will be at least $T$ cards required for the RHS .

If the PROCEDURE is used separately, then all these quantities are input parameters (with the same names as above).

A complete sample input is given by,
A $\left\{\begin{array}{cccccc}3 & 3 & 1 & 0 & @ 14 & 0.001 \\ 1.3 & 2 & & -5 & & \\ 4 & 1 & 0 & & \\ -1 & -1.3 & @ 3 & \\ \text { RHS }\left\{\begin{array}{cccc}1 & 2 & 2.1\end{array}\right.\end{array}\right.$

Output
All the matrices printed out by the program will have the following format:

Eight columns per line, each number in floating point with 6 significant digits. If the matrix is more than eight columns wide, then successive blocks will be printed in new pages. All the rows are printed together.

The output is described now in the order in which it will occur.
First the matrix A is printed out.
Then, if $O P C=0$, the right-hand sides are printed out.
Norm of $(B C-A)$.
The residuals $\| A x_{m}^{(i)}-$ RHS $^{(i)}\|\|, A x_{b}^{(i)}-R H S{ }^{(i)} \|$.
If $O P C=1$, then the matrix pseudoinverse is printed out with the format explained above; also in this case the non-zero rows of the matrix $A^{\#}$ are printed, each of them with a heading: ROW NUMBER.... .

If $O P C=0$, then instead of these two last matrices, the minimum and basic solutions are printed out. As an example, we give the output for the problem:

$$
\left(\begin{array}{ll}
9 & 21 \\
21 & 49
\end{array}\right) \quad x=\left(\begin{array}{ll}
1 & 0 \\
0 & 1
\end{array}\right)
$$

PSEUDOINVERSION OF THE MATRIX A . A IS $2 \times 2$.

$$
\begin{array}{ll}
9.00000 @+00 & 2.10000 @+01 \\
2.10000 @+01 & 4.90000 @+01
\end{array}
$$

[PAGE]
NORM OF (BC - A) $\quad 2.37582 @-12$
RESIDUAL FOR XM

$$
9.19145 @-01 \quad 3.93919 @-01
$$

RESIDUAL FOR XB

$$
9.19145 @-01 \quad 3.93919 @-01
$$

[PAGE]
MATRIX APSEUDOINVERSE

| $2.67532 @-03$ | $6.24314 @-03$ |
| :--- | :--- |
| $6.24381 @-03$ | $1.45794 @-02$ |

[PAGE]
MATRIX ADAGGER
ROW NUMBER 1

$$
1.72461 @-02 \quad 4.02332 @-02
$$

END OF THE RUN

The PROCEDURE PSEUDOINVER.
The call for this PROCEDURE is,
PSEUDOINVER (M, N, TI, OPC, SUPER, ORTP, A, RHS, EST, NXM, NXB,
APSEUDO, ADAGER, COF, XM, XB);

The first 8 parameters are input parameters and they have been described before. The only detail needed is: A(double real array $[0: M, O: N]), \operatorname{RHS}[0: M, O: T I] ;$

OUTPUT PARAMETERS:
$\operatorname{EST}$ (real) Contains $\|\mathrm{BC}-\mathrm{A}\|$.
NXM, NXB (single real arrays [O:TI]). They contain the residuals
$\left\|A X_{m}-R H S\right\|$ and $\| A X_{b}$ - RHS $\|$ respectively.
APSEUDO, ADAGER (Double real array $[0: N, O: M])$
They contain the pseudoinverse of $A$ and the matrix $A^{\#}$.
COF (Single integer array $[0: N]$ ).
If $\operatorname{COF}[I]=0$ then both, the $I^{\text {th }}$ row of $A^{\#}$ and $X_{b}$ are different from zero, otherwise they are zero and that means the program has decided that the corresponding columns in $A$ were linearly dependent with respect to the current basis.
$\mathrm{XM}, \mathrm{XB}$ (double real arrays, $[0: N, 0: T I]$ )
They contain the minimum and basic solutions.
IV. Test Problems.
a) Square segments of the Hilbert matrix have been tried, sizes varying between 3 and 10 .

For $5 \leq \mathrm{n} \leq 10$ the rank found in each case was 4 . The norm of the pseudoinverses remained below $10^{3}$ while for the true pseudoinverse (the inverse in these cases) the norms ranged between $10^{5}$ for $n=5$ and $10^{13}$ for $n=10$. The norm, $\|A-B C\|$ was around $10^{-5}$ for all cases. As is well known, the ill-conditioning of the Hilbert matrix segments increase with their dimension. However, because of the smoothing property of the method a bounded and reasonably accurate representation for the pseudoinverse was always obtained.
b) Eighteen random matrices with random dimensions varying between $I$ and 25 were generated and pseudoinverted. The norm $\|A-B C\|$ was always below $10^{-9}$ and the ranks were always found to be equal to $\min (m, n)$.
c) Given three random integers $m, n$ and $r$ in the interval [1, 25]
a routine generated two random matrices, $L(m \times r)$ and $R(r \times n)$. Multiplying them we obtained a matrix $A(m \times n)$ with rank at most equal to $r^{(1)}$. With 20 matrices generated in this way, the results were similar to b). In every case the rank $r$ was correctly determined. For most of these cases the rank $r$ was less than $\min (m, n)$, and of course was unknown for the program.
(1) This test was suggested by Professor Gene H. Golub.
d) For each pair of values ( $m, n$ ) several random matrices were generated and pseudoinverted. Average values of $\|A-B C\|$ for these matrices with $m=10,20,30$ and $n=10,20,30$ are shown in Table I. For the same problems, average computation time on the Burroughs B5000 at Stanford Computation Center are shown in Table II.

In all these matrices the rank was the maximum possible, i.e., rank = $\min (m, n)$ and it was properly determined by the program.

TABLE I

| $m$ | 10 | 20 | 30 |
| :---: | :---: | :---: | :---: |
| 10 | $5 \times 10^{-9}$ | $9 \times 10^{-9}$ | $4.5 \times 10^{-8}$ |
| 20 | $3 \times 10^{-10}$ | $4 \times 10^{-8}$ | $2.9 \times 10^{-7}$ |
| 30 | $5.8 \times 10^{-10}$ | $6.9 \times 10^{-9}$ | $2.6 \times 10^{-7}$ |

$\|A-B C\|$

TABLE II

| $m$ | 10 | 20 | 30 |
| :---: | :---: | :---: | :---: |
| 10 | 7.6 | 13.9 | 20.7 |
| 20 | 16.5 | 49 | 91 |
| 30 | 27.3 | 92.5 | 180.6 |

Comp. time in seconds

For a $40 \times 40$ matrix the answers were:

$$
\begin{array}{ll}
t=413 \mathrm{sec} . & \|\mathrm{A}-\mathrm{BC}\|=2.7 \times 10^{-7} \\
\text { rank }=40 . &
\end{array}
$$

e) A common problem in many branches of applied sciences is the least squares fit, and is therefore one of the most important applications for this program. A related feature of the program is that, by ordering the variables, the user will be able to test their independence and eventually to decide if his model is appropriate to the phenomena being investigated. This is done by ordering
the matrix A so that the first coefficients correspond to the more important variables. The program will attempt to use these columns first to form the basis B . The necessity for such an ordering is clear from the fact that if we have $n$ columns in A and the subspace spanned by these columns has dimension ( $\mathrm{n}-\mathrm{p}$ ) then we can construct with these columns as many as ( $n-p$ ) linearly independent sets. In Figures II and III are shown the results obtained by running the program with least squares type problems. Again the elements of the matrices were generated randomly. Fig. II shows computation times on the B5000 for different values of $m$ and $n=5,10$. Fig. III shows the norm $\|A-B C\|$ for the same problems.
f) Matrices with exact known inverses were tried obtaining good results and accuracy. Of course this program should not be used to invert a matrix which is known to be nonsingular and wellconditioned, because it will be around four times slower than an efficient matrix inverter. The program has also been used to obtain the pseudoinverse of singular and almost singular matrices steming from the discretization of integral equations of the first kind, and problems in pattern recognition.


FIGURE II


FIGURE III

## V. Storage Requirements.

As all the array declarations are dynamical, the amount of storage depends on several parameters. If $M, N, T$ are as before, and $R$ is the final rank (number of accepted columns) then an estimate for the storage used in the PROCEDURE PSEUDOINVER is,

$$
\text { Storage } \cong N^{2}+5 M N+M R+2 N R+2 N T+\max \left(R^{2}, M N, M T\right)
$$

the last term is present because in the PROCEDURE GARBG we have several independent blocks, and the storage corresponding to certain arrays is not simultaneously used.

If, as usual, $R$ is not known, then it can be replaced by $\min (n, m)$. If the complete program is used then additional storage is needed,

$$
\text { Addit. storage } \cong 3 M N+M T+2 N T
$$

Computer time rapidly increases when abusive use of the drum is made. From the experience obtained with the test problems, it is suggested that the total storage be less than 40,000 words.

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AN EXTENDED ALGOL PROGRAM TO COMPUTE THE PSEUDOINVERSE OF AN $M \times N$ REAL MATRIX AND OTHER RELATED QUANTITIES.

BEGIN COYMENT PSEUDOINVERSE OF A MXN MATRIX OF UNKNONN RANK; INTEGER $Y, N, T$ I,I,J ; REAL SUPES.EST,TPD,ORTP; BOOLEAN JPC ; LAREL OVER,FIU;

```
COMMENT DRIVER PROGRAM. FIRST PARAMETERS ARE READ IN,
                AND USED FOR FURTHER DYNAMICAL ARRAY DECLARATIONS;
```

OVER: READ (M,N,TI,OPC,SUPER,ORTP) [FIU];
BEGIN INTEGER ARRAY COF[O:N];
ARRAY A[O:Y,O:N],RHS[O:M,O:TI],XM,XB[O:N,O:TI],NXY,NXB[O:TI],
APSEUDO,ADAGER[O:N,O:M]; LABEL NOPR,NOPRI;
FORMAT DRYAT(( BE14.5)//1),
TITI("PSEUOOINVERSION OF THE MATAIX A"///"A IS",I3,"x",I3/),
TIT7("VORY OF (BC"A)"//X3,E15.5/"RESIDUAL FOR XY"/(8E15.5/)),
TIT8("YATRIX A PSEUDOINVERSE"/),TIT9("MATRIX A DAGGER"/)
TITIO (X6, "XM"/), TIT20(//X6, "XB"/) , TITL38(/"ROW VUMBER", I 3/)
TIT77(/"RESIDUAL FOR XB "/(BE15.5/)),SOL(8E15.6/),
ENDE(//"END OF THE RUN*//X15,"***********"////))
PROCEDURE PRT(A,M,N) ;
INTEGER $M, N$ : ARRAY $A[0,0]$;
COMMENT PRT PRINT DUT THE MXN MATRIX A;
BEGIN FJRMAT TITL46(/ 8E14.5); INTEGER SE,K,R!
SE * NDIV 8 ; K + NMDD 8;
FOR R+O STEP 1 UNTIL SE-1 DO
BEGIN FOR I+1 STEP 1 UNTIL M DD
WRITE (TITL46,FOR J+1 STEP 1 UNTIL 8 DO A(I. $8 \times R+J Y)\}$
WRITE ([PAGE])
END: IF KOO THEN FDR I + 1 STEP 1 UNTIL M DO

WRITE ([PAGE])
END PRT:
PROCEOURE PSEUDOINVER (M,V,TI,SUPER,OPC,A,RHS,ORTP,EST,NXM.
VXB,APSEUDO, ADAGER, (OF, XM, XB);
INTEGER Y,N.TI ; INTEGER ARRAY COF[OJ; BOOLEAN OPC;
REAL SUPER,EST,ORTP ;
ARRAY A,RHS, APSEUDD,ADAGER, XM, XB[0,O],NXM,NXB[O];
COMMENT PSEUDOINVEF COMPUTES THE PSEUDOINVERSE OF A MXN MATRIX A.
AND DTHER RELATEO QUANTITIES. THE ESPECIAL WAY OF ROUNDING-OFF
AFTER DOUBLE PRECISIDN OPERATIDNS IS DUE TO
YR. PETER RUSINGER AND PROF. GENE GOLUB;
BEGIN IVTEGER J,CONT,Q,K,T,BUENO,R,I,PE,MA; BOOLEAN SUITCH;
ARRAY BQ, AN[O:M,O:N], INVQ[O:N, O:N],NRHS,UPI, DOPI[O:TI],
G.UO,SAV[O:N],XI,X2[0:N,O:TI],BPS,API,ADI[O:N,O:M];
REAL CLUF,ALFAQ, BEQ,AL,SUPALF,B,NXBI,NXMI,AAA,BBB,CCC,
UPII, DOPII,ESTI,ASO,SUM,ES,PERTUB,ESTIM,TPD,MINIR;
MA \& IF M<N THEN N ELSE M:
BEGIN ARRAY TRUC,TU,VQ,TEMPIO:MAJ; LABEL SECNO,RFIN,
NONES, LOP, TRES, CUATRO,MAIS,CAS,FINI, OTRA,FORCED;
COMMENT TRMAVC,MATRIMUL,MULTIVECPESCPTRANSP AND VECSUM ARE
PROCEDURES PERFORMING MATRIX AVD VECTOR OPERATIONS,
SOME OF THEM IN DOUBLE PRECISION;
PROCEDJRE TRMAVC $(A, V, I, J, M, N)$;
ARRAY $A[0, O], V[0] ;$ INTEGER I,J,M,N;
BEGIN INTEGER K;
IF I=0 THEN FOR K+1 STEP 1 UNTIL M DO V\{イ]+A[KOJ]
ELSE FOR K+1 STEP 1 UNTIL N DO V[K]* A[IAK]
END TRMAVC;

```
    PROCEDJRE MATRIMUL (A,B,C,P,Q,R);
                            ARRAY A,B,C[O,O] ;INTEGER P,Q,R ;
    BEGIN INTEGER I,J,K ;REAL AC,BC;
        FOR I+1 STEP 1 UNTIL P DO FOR J+1 STEP 1 UNTIL R DO
        BEGIN AC&BC+O; FOR K+1 STEP 1 UNTIL Q DO
            DOUBLE(A[I,K],O,B[K,J],O,X,AC,BC,+,4,AC,BC):
            C[I:J] & AC+BC&AC[1:1:8]/5.49755813891811
        END
    END MATRIMUL:
PROCEDJRE MULTIVEC (A,VI,V2,P,Q)S
                            ARRAY A[0,O],VI,V2[O] IINTEGER P,Q;
    BEGIN INTEGER I,J; REAL AC,BC;
        FOR I+I STEP 1 UNTIL P DO
        BEGIN AC+3C+0; FOR J+1 STEP 1 UNTILQ OO
            DOUBLE (A[I,J],O,VI[J],O,X,AC,BC,+,+,AC,BC))
            V2[I]* AC+9C&AC[1:1:8]/5.49755813891011
        END
    END MULTIVEC;
PROCEDJRE ESC(A,B,C,P);
                                    ARRAY A,B[O] ;REAL C ; INTEGER P;
    BEGIN INTEGER I;
        C+O; FOR I+I STEP I UNTIL P OD C* A[IIX 3[I]+C
    EVD ESC;
PROCEDURE TRANSP (A,B,P,Q);
            ARRAY A.B [0.0]; INTEGER P,Q ;
    BEGIN INTEGER I,J;
        FOR I+I STEP I UNTIL P DO
        FOR J+1 STEP I UNTIL Q DO B[J.I] * A[I,J]
    END TRANSP;
PROCEDJRE VECSUM (A,B,C,ALF,BET,N);
                        ARRAY A,E,C[O]; REAL ALF,BET ;INTEGER N;
        BEGIN INTEGER I;
        FOR IHI STEP I UNTIL N DO C[IIJALIJXALF+B[IJX BET
    END VECSUM ;
PROCEDJRE DSEUDD (NQ,ALFQ,UQ,Q);
                            ARRAY NQ[O,O],UQ[O]; REAL ALFQ; INTEGER O ;
COMMENT GIVEN(BQ"BQ) INVERSE, PSEUDO CONSTRUCT (B(Q+1)HB(Q+1))
        INVERSE;
    BEGIN REAL A; INTEGER I'J;
        ALFQ + 1/ALFQ;
        FDR I+I STEP 1 UNTIL Q DO FOR J+I STEP I UNTIL Q DO
                DOUBLE(ALFQ,O,UQ[I],0,X,UQ[J],0,X,NQ[I,J],O,+,+,
                    NQ[I;J],A); Q+Q+1; UQ[Q]+ -1;
        FOR J+I STEP I UNTIL Q DO
        NQ[J,Q]+NQ[Q,J] * - ALFQ x UQ[J]
    END PSEUDO;
PROCEDURE GARRG(M,N,T,TI,COF,BQ,G,RHS,BPS,A,NRHS,AAA,
                                    NXM,NXB,NXM1,NXB1,APSEUDO,ADAGER,XM,XB,EST)I
                                    REAL NXM1,NXBI,EST,AAA; INTEGER N, Y,T,TI;
                INTEGER ARRAY COF[O];
                ARRAY XM,XB,APSEUDO,ADAGER,BQ,RHS,BPS,A[O,OJ.
                                    NXB,NXM,G,NRHS[O];
COMMENT GIVEN THE BASIS BQ: A PSEUDOINVERSE, A DAGGER, XM, XB,
        NXY, NXB, AND NORM OF (A=BQC) ARE COMPUTEDS
        BEGIN INTEGER I,Q,J,R,MA ; REAL B,PER,ALFAQ:
```

```
                            ARRAY C[O:T,O:N], BQL[O:M,O:T],UQ[O:N];
    IF MSN THEN MA+N ELSE MA +M;
    BEGIN ARRAY AN[O:T,O:N];
        BEGIN ARRAY INVQI[O:T,O:T],TU,TEMP[0:MA];
COMMENT A DAGGER IS CALCULATED;
        FOR I+1 STEP I UNTIL N DO
        BEGIN Q + COF[I];
            IF Q*O THEN FOR J+1 STEP 1 UNTIL M OO
            BEGIN BQI[J,Q] * BQ[J,Q]/G[I];
                ADAGER[I,I]+ BPS[Q,J]+ BPS[Q,J]\times G[I];
            END
        END;
COMMENT C AND C-PSEUDOINVERSE ARE CALCJLATED;
        MATRIMUL(BPS,A,C,T,M,N);
        TRMAVC(C,TU,1,I,T,N): ESC(TU,TU,B,N)&
        INVQ1[1,1]+1/B;
        FOR Q* 2 STEP 1 UNTIL T DO
        BEGIN R& Q-1; TRMAVC(C,TU,Q,Q,T,N)S
            MULTIVEC(C,TU,TEMP,R,N);
            MU!TIVEC(INVQI,TEMP,UQ,R,R);
            FOR I*I STEP 1 UNTIL N DO
            BEGIN PEq+ 0;
                FOR J+1 STEP 1 UNTIL R DO
                PER+ PER+C[J.I) x UQ[J]; TEMP[I) * PER
                    END:
                    VECSUM(TU,TEMP,TEMP,1,-1,N):
                    ESC(TEMP,TEMP,ALFAQ,N);
                    PSEUDO(INVQL,ALFAQ,UQ,R)
                ENO; MATRIMUL(INVQI,C,AN,T,T,N);
        ENO;
        BEGIN ARRAY BQC[O:MA,O:N],
COMMENT NORM OF (A-BC) IS COMPUTED;
        TRANSP(AN,BQC,T,N) ;
        MATRIMUL(BQC,BPS,APSEUDO,N,T,M);
        MATRIMUL(BQI,C,BQC,M,T,N); EST + O&
        FOR I+1 STEP 1 UNTIL M DO
        BEGIN PER+ O;
                            FOR J+I STEP I UNTIL N DO
                            PER& PER+ABS(BQC(I:J]=A{[:J])}
                            IF PERZ EST THEN EST * PER
                END
        END
        END:
    EST + EST/AAA;
COMMENT THE MINIMUM AND BASIC SOLUTIONS ARE COMPUTEOS
    MATRIMUL(APSEUDO,RHS,XM,N,M,TI):
    MATRIMUL(ADAGER,RHS,XB,N,M,TI);
    BEGIN ARRAY AN[O:M,O:TI]:
COMMENT THE RESIDUALS FOR THESE SDLUTIONS ARE COMPUTEDS
        MATRIMUL (A,XM,AN,M,N,TI);
        FOR J+1 STEP 1 UNTIL TI DO
        BEGIN NXM1+0;
            FOR I+1 STEP 1 UNTIL M DO
            NXM1 +(AN[I,J)-RHS[I,N])*2+NXM1:
            NXM1* SQRT(NXM1):NXM[J]*NXM1/NRHS[J]
```

```
    ENO;
    MATRIMJL(A,XB,AV,M,N,TI):
    FOR J+1 STEP 1 UNTIL TI DO
        BEGIN NXB1+0;
            FOR I*1 STEP 1 UNTIL N OO
            NXB1+(AN[I,J]mRHS[I,J])*2 + NXB1;
            NXB1* SQRT(NXB1); NXB[J]+ NXB1/NRHS[J]
        END;NX31+NXM1 + 0;
        FOR I+1 STEP 1 UNTIL TI DO
        BEGIN NXBI * NXBI + NXB[I]*2;
            NXM1 * NXMI+NXM[I] *2
        ENO; NXM1+SQRT(NXM1); NX81+ SQRT(NXB1);
            END;
        EVD GARBG;
COMMENT PRJCEDURE PSEUODINVER BODY;
    MINIR +Q-20; }\triangleAA+CCC+0
COMMENT NORM JF A ANO NORM OF THE RHS;
    FOR J+1 STEP I UNTIL N DO FOR I+1 STEP 1 UNTIL M DO
    BEGIN BBB+ ABS(A[I,J]); IF BBB>AAA THEN AAA+BBB
    EVO ; FOR J+1 STEP 1 UNTIL TI DO
    BEGIN CCC+O; FOR I+1 STEP I UNTIL M OO
            CCC+CCC+RHS[I,J]* 2; CCC+ SQRT(CCC);
            VRHS[J]* IF CCC>1 THEN CCC ELSE 1;
        EVD; IF AAA<1 THEN AAA+1;
        FOR I+1 STEP I UNTIL N OO
        BEGIN COF[I]+ 0;
        FOR J+1 STEP I UNTIL M DO ADI[I,JJFADAGER[I,J]+ O;
    END ;
        COMMENT THE MATRIX A IS NORMALIZED AND STORED ON AN,
                G CONTAINS THE NORMALIZING COEFFICIENTS;
    FOR J&I STEP 1 UNTIL N DO
    BEGIN TRMAVC(A,TU,O,J,M,N):
        ESC(TU,TU,CLUF,M);
        G[J]+IF CLUF > 1.0 THEN 1.0/SQRT(CLUF) ELSE 1.0:
    EVD ; FOR I+1 STEP 1 UNTIL M DO
    BEGIN FOR JHI STEP 1 UNTIL N DO
        AN[I,J] + A[I,J]\timesG[J]
    EVD;
        COMMENT THE CONSTRUCTION OF A BASIS OF STRONGLY
            INDEPENDENT VECTORS IS STARTED:
    CONT+1; SUPALF+ 0; Q+K+T+1;
    COF[1]+1; INVQ[1,1]+ 1; SUITCH+ FALSE ;
    FOR I&1 STEP 1 UNTIL M OO BQLI:I]+ AN[IOII:
COMMENT SEARCH FOR INDEPENDENT COLUMNS OF A. WHEN THE COLUMNS
        ARE EXHAUSTED AN EXIT IS PROVIDED TO LABEL FINI. IN CONT
        A RECORD IS KEPT ON THE WAY IN WHICH COLUMS ARE ACCEPTEDS
    LOP: IF Q=N THEN GO TO FINI;
    T+K; Q+Q+1; K+K+1;
COMMENT PRJJECTION OF A COLUMN OF AN ON THE ORTHOGOVAL
            SUGSPACE DF BQ:
CAS: TRMAVC(AN,VQ,O,Q,M,N);
    FOR I+1 STEP I UNTIL T DO
    BEGIN ALFAQ* O;
                            FOR J+I STEP I UNTIL M DO
                            ALFAQ* ALFAQ+BQ[J,I]XVQ[J]; TEMP[I]+ ALFAQ
```

```
    EVD;
    MULTIVEC:INVQ,TEMP,UQ,T,T);
    MULTIVEC(BQ,UQ,TEMP,M,T);
    VECSUY(VQ,TEMP,TEMP,1,"1,M);
    ESC(TEMP,TEMP,ALFAQ,M);
    IF SUITCH THEN GO TO TRES;
COMMENT FIPST TEST FOR ACCEPTANCE AS AN INDEPENDENT COLUMN;
    IF ALFAQ S ORTP THEN GO TO NONES;
    IF COVT=2 THEN CONT+ 3;
COMMENT COVSTRUCTION OF B(O+1);
    PSEUDO (INVQ,ALFAQ,UQ,T);
    FOR I+1 STEP 1 UNTIL M DD BQ[IOK]+ VQ[IJ;
    COF [Q]+K; GD TO LOP;
NOVES: COF[Q] + O; K+K=1;
    IF COVT & 3 THEN
    BEGIN CONT+2; GO TO TRES;
    EVD ; GD TO LOP;
COMMENT IF CONT\notZ THEN THE REJECTED COLUMNS ARE REVISED IN DROER
    TO TAKE THE MOST INDEPENDENT WITH RESPECT TO THE BASIS BQ.
        COVT=1 MEANS THAT A!L THE CDLJMNS HAVE BEEN TAKEN IN THE
        FIRST SWEPT. CONT=3 MEANS THAT A COLUMN HAS BEEN REJECTED
        ANO LATER ON.ANOTHER HAS BEEN ACCEPTED;
OTRA: Q+ 2; SUPALF+ O; BUENO& O;
MAIS: IF Q=N+1 THEN GO TO CUATRO;
    IF COF[Q]# O THEN
    BEGIN O+ Q+1; GO TO MAIS;
    END ; GO TO CAS;
TRES : IF ALFAQ \geq SUPALF THEN
    BEGIN SUPALF + ALFAO;
            FOR I+1 STEP I UNTIL M OO TRUCIIJ* VQ[IJ:
            FOR I+1 STEP I UNTIL T DO
            SAV[I]+ UQ[I]; BUENO & Q
    EVD ; IF CONT=2 THEN GO TO LOP ;
    IF Q=N THEN GO TO CUATRO;
    Q+ Q+1; GO TO MAIS;
COMMENT IF THE PROJECTIDN OF THE SELECTEO COLUMN IS LESS THAN O-2O
    THEN SAV IS REJECTED AND WE FINISH;
CUATRO: IF SUPALFS MINIR THEN GO TO RFIN;
    AL +SUM + O;
COMMENT THE NORM OF (B(Q+1)"B(Q+I)) INVERSE IS ESTIMATED,AND ITS
        VALUE IS CONTROLLED;
    FOR I+1 STEP I UNTIL T DO
    BEGIN FOR J+1 STEP I UNTIL T DO
                SUM +SUM + ABS(INVQ[I,J])S
                IF SUM>AL THEN AL+SUM
    END ;
    ESTIM * AL+(SQRT(T)+1.0)/SUPALF ;
    IF ESTIM Z SUPER THEN GO TO RFIN:
COMMENT SAV HAS PASSED THE TESTS OF SECTION 2,C). NJW IS USED
            TEVTATIVELY IN B(Q+1) TO SEE IF THE RESIDUALS DIMINISHS
FORCED: PSEJDO(INVQ,SUPALF,SAV,T);
    COF[RUENO]* T ;
    FJR I+1 STEP I UNTIL M DO BQ[I,T]* TRUC[I];
    COMMENT WE CONSTRUCT NOW B-PSEUDO,C,A-PSEUDO AND ADAGGERS
FINI : FOR I+1 STEP I UNTIL T DO FOR J+1 STEP I UNTIL M DO
```

```
    BEGIN ES&O; FDR PE+1 STEP I UNTIL T DO
        ES + ES + INVQ[I,PE] x BQ[J,PE]; BPS[IPJ] +ES
COMMENT AS NE WAVT TO COMPARE RESULTS FOR TWO OIFFERENT BASES,
        SUITCH PROVIDES A NAY TO DECIDE THE CALL OF GARBG:
        EVD; IF SUITCH THEN GO TO SECND ;
        GARGG (M,V,T,TI,CDF,BQ,G,RHS,BPS,A,NRHS,AAA,
                    NXY,NXB,NXM1,NXB1,APSEUDD,ADAGER,XM,XB,EST);
        IF T=N THEN GO TO RFIN; SUITCH & TRUE;
        IF CJNT = 2 THEN
        BEGIN CONT * 1; GO TO CUATRO;
        EVD; GOTD OTRA;
SECND: GARZG (M,V,T,TI,COF,BA,G,RHS,BPS,A,NRHS,AAA,
                UPI,DOPI,UPII,DOPII,API,ADI,X1,X2,ESTII;
COMMENT VON THE TEST OF SECTION 2,D) IS MADE;
        IF NXBI\geq DOPII AND NXMI\geqUPII THEN
        BEGIN IF NOT DOC OR EST\geq ESTI THEN
COMMENT IF SAV IS ACCEPTED THEN ALL THE JSEFUL QUANTITIES
        ARE SHIFTED;
            3EGIN NXMI+UPII; NXBI* DOPII; EST&ESTI;
                FOR I+1 STEP 1 UNTIL N DO
                8EGIV FOR J+1 STEP I UNTIL M DO
                    BEGIN APSEUDO[I,J]* API[I,JJ;
                        ADAGER[I,J]+ADI[I;J]
                            END: FOR J+1 STEP I UNTIL II DO
                            BEGIV XM[I;J]+XI[I;J]; XB[I;J]+ X2[I;J];
                                    NXM[J]+UPI[J]; NXB[J]&DOPI[J];
                                    END;
                                    END : IF T=N THEN
                BEGIN BUEND+O ; GO TO RFIN
                END ; GO TO OTRA
            END
        EVO;
RFIN: COF[BUENO]+ 0;
        END
    END PSEJDIIVVER;
COMMENT BOJY OF THE DRIVER PROGRAM. THE INPUT-DUTPUT AND THE CALG
    IF PSEUDOINVER ARE INCLUDED:
    FOR I+1 STEP 1 UNTIL M DO
    READ(FOR JHI STEP I UNTIL N DO A[I,JI);
    WRITE( [PAGE]); NRITE(TITI,U,N); PRT(A,M,V);
    IF NOT OPC THEN FOR I & STEP 1 UNTIL TI DO
    READ( FOR JN1 STEP 1 UNTIL Y DO RHS[J.IJ)
    ELSE FOR I+1 STEP I UNTIL M DO FOR J+1 STEP 1 UNTIL M DO
    RHS[I,J]+ IF I=J THEN I ELSE O ;
PSEUDIIVVER(M,N,TI,SUPER,OPGNA,RHS,ORTP,EST,NXM.
    NXB,APSEUDO,ADAGER,COF,XM,XB);
    WRITE(TITT,EST,FOR I & STEP 1 UNTIL TI DO NXM[IJ)&
    WRITE(TITT7, FOR I+1 STEP 1 UNTIL TI DO NXB[IJ);
    IF OPC THEN
    BEGIV NPITE([PAGE]) ; WRITE(TITB);
        PRT(APSEUDO,N,M); WRITE (TITQ);
        FOR I+1 STEP 1 UNTIL N OO
        BEGIN IF COF[I]=0 THFN GO TO NOPR;
        WRITE (TITL38,I);
        WRITE (PRMAT,FOR J+1 STEP 1 UNTIL M DO ADAGER[I:JJ) ;
```

NOPR: END END


BEGIN WRITE([PAGE]); WRITE(TIT10); FOR I 1 STEP 1 UNTIL $V$ DO WRITE(SOL,FQR J+1 STEP I UNTIL TI DO XM[I.JJ): WRITE (TIT20); FOR I\&I STEP 1 UNTIL N DO BEGIN IF COF [I]=O THEN GO TO NOPRIS WRITE(TITL3B,I) NPITE(SDL,FOR J+1 STEP 1 UNTIL TI DO XBEI,JJ)
NOPR1:
COMMENT END;
JUST BY ADOING NEW SETS OF DATAS MORE PROBLEMS CAN BE RUN: END: WRITE(ENOE); GO TO UVER;
END ;
FIU:
END.

