

NBER WORKING PAPER SERIES

THE SINGULAR VALUE ANALYSIS
IN MATRIX COMPUTATION

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Working Paper No. 46

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July 1974

Preliminary: not for quotation

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This report has not undergone the review accorded official NBER publications; in particular, it has not yet been submitted for approval by the Board of Directors.

*NBER Computer Research Center. Research supported in part by National Science Foundation Grant GJ-1154X3 to the National Bureau of Economic Research, Inc.

Abstract

This paper discusses the robustness and the computational stability of the singular value decomposition algorithm used at the NBER Computer Research Center. The effect of perturbations on input data is explored. Suggestions are made for using the algorithm to get information about the rank of a real square or rectangular matrix. The algorithm can also be used to compute the best approximate solution of linear systems of equations in the least squares sense, to solve linear systems of equations with equality constraints, and to determine dependencies or near dependencies among the rows or columns of a matrix.

A copy of the subroutine that is used and some examples on which it has been tested are included in the appendixes.

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The singular value decomposition of a matrix is one of the most elegant algorithms in numerical algebra for exposing quantitative information about the structure of a system of linear equations. It can be used to get information about the rank of a square or rectangular matrix, to compute the best approximate solution of a linear system of equations in the least squares sense, to solve systems of linear equations with equality constraints, and to determine dependencies or near-dependencies among the rows or columns of a matrix. Occasionally the singular value decomposition is used in the iterations of linear systems that tend toward the solution of nonlinear systems of equations. The condition number of a matrix with respect to the solution of a linear system of equations is a by-product of the singular value decomposition as is the production of the pseudo-inverse and the solution of homogeneous systems of equations.

The condition number of a matrix with respect to the solution of a linear system of equations shows how well the vector x is defined by the transformation $Ax=b$. The condition number $\kappa(A)$ of the nonsingular matrix A is the ratio $\frac{\sigma_{\max}}{\sigma_{\min}}$ where σ_{\max} and σ_{\min} are, respectively, the maximum and minimum singular values of A (i.e., the non-negative square roots of the eigenvalues of $A^T A$ where A^T denotes the transpose of A). For example, if $\kappa(A)=10^6$, a perturbation of 2^{-20} in the elements of A can change the computed solution \hat{x} by a factor of $2^{-20} \cdot 10^6$, that is to say, even the leading digit may be changed. For a more rigorously detailed explanation, see [9].*

*Numerals in square brackets refer to entries in the Reference section, p. 15.

In the discussion that follows, we seek to compute directly the best approximate solution to the possibly over-determined or under-determined system of equations

$$Ax = b.$$

The singular value decomposition is used to obtain this solution. Frequently a user, or a problem originator, poses a problem from which he wants to obtain a solution vector x in the sense of least squares from the system of equations

$$A^T Ax = A^T b.$$

Possibly he thinks the information he needs comes from the solution

$$x = (A^T A)^{-1} A^T b.$$

Classically, (1) if the data matrix A and the vector b are exact (that is to say, there is no uncertainty in the data A and b), (2) if the precision of the arithmetic of the machine is such that $A^T A$ can be formed and stored exactly, and (3) if $A^T A$ is of full rank, the solution x could be obtained from $(A^T A)^{-1} A^T b$. However, given that these three conditions are seldom attainable in practice, the solution should not be computed in this way because of the extra precision that is required. Furthermore, unless there is a priori exact information known about the rank of A , the solution x cannot be obtained from the pseudo-inverse of A with any more

authenticity than from $(A^T A)^I$. That is to say the rank should be determined during the course of computing the singular value decomposition. Reliable information about rank deficiency cannot be obtained from triangular factorization.

Sylvester wrote an article on the singular value decomposition of real $n \times n$ matrices in 1889 [10]. Eckert and Young extended the work to general matrices in 1936 [1]. The definitive paper on calculating the singular value decomposition was written by Golub and Kahan [2]. Though the paper was published in 1965, it is fair to say that its use as a robust tool of mathematical software is recent and, as of now, is not very widespread (see [4] and [5]).

The singular values of the matrix A and the non-negative square roots of the eigenvalues of the symmetric matrix $A^T A$ are mathematically equal, but may be different computationally. Singular values correct to working accuracy for the matrix A can often be computed when certain small eigenvalues cannot be computed for $A^T A$. This fact is not startling. It is caused by the perturbation of an exact $A^T A$ introduced in the multiplication of A^T by A . There are many examples of such matrices, one of which is illustrated in [9], assuming a 4-decimal-place machine, as

$$A = \begin{bmatrix} 1.005 & 0.995 \\ .995 & 1.005 \end{bmatrix}$$

having singular values 2.0 and .01. The matrix $A^T A$ in 4-decimal arithmetic is

$$A^T A = \begin{bmatrix} 2.000 & 2.000 \\ 2.000 & 2.000 \end{bmatrix}$$

with eigenvalues 4.0 and 0.0. Attrition in forming $A^T A$ has obscured all information about the smaller singular value.

The subroutine MINFIT, using the notation in [2], reduces the system of equations

$$Ax = b$$

where A has m rows and n columns (m can be less than, equal to, or greater than n) to the form

$$U \Sigma V^T x = b$$

giving $\Sigma V^T x = U^T b$.

The columns of V are the orthonormal eigenvectors of $A^T A$. The transformation $U^T b$ is formed directly -- U is not computed explicitly. The columns of U are the orthonormal eigenvectors of AA^T . If one needs the explicit columns of U he should append the identity matrix I_m to the right-hand side b. There is no restriction, at the subroutine level, on the number of columns of b; it can be zero.

The diagonal matrix, Σ , contains the singular values of A. The transformations used to obtain the decomposition preserve unitarily invariant norms, thereby assuring that the norm of Σ is that of A. The diagonal elements of Σ , when ordered, are $\sigma_1 \geq \sigma_2 \geq \sigma_3 \dots \geq \sigma_n \geq 0$. MINFIT does not order the singular values. Given information about the certainty of the data A and b, one can choose the best approximating matrix A_r of full rank that is nearest, in the norm sense, to the matrix A. From A_r the best candidate solution x for $Ax=b$ can be computed. If σ_r is chosen such that

$$\Sigma V^T x = U^T b = c$$

from which

$$x = V \Sigma^+ c.$$

Various candidate solutions x can be provided by different choices of a rank tolerance to fix σ_r . See [6], chapters 25 and 26.

For suitably chosen σ_r , consider those columns of V associated with $\sigma_{r+1}, \sigma_{r+2}, \dots, \sigma_n$ as V_v , namely the columns of V that span the null space of A . Then

$$AV_v = 0.$$

When such columns V_v exist, they constitute the non-trivial solutions of the homogenous system of equations

$$AX = 0.$$

The elements of the columns of V can be inspected to reveal dependencies or near dependencies among the columns, i.e., the variables of the coefficient matrix A . Analogously, the columns of U can reveal dependencies among the equations, i.e., the rows of A .

In using MINFIT, and providing it to other users, we are concerned with three distinct but related items, (1) the stability of the algorithm from the standpoint of numerical algebra, (2) the robustness of the mathematical software that implements the algorithm, and (3) the documentation that provides information on the use of the mathematical software.

The numerical stability of an algorithm usually means that the solution that is computed is the exact solution of a neighboring problem and that the neighboring problem can be defined in the sense of a backward error analysis. Such analysis for the singular value decomposition has been

published in [2], [11], [12], and [13]. The singular value decomposition is stable in the sense that the computation of eigensystems of Hermitian matrices is stable. In general, we expect

$$\frac{\|A - U\Sigma V^T\|}{\|A\|}$$

to be the order of machine precision, as is corroborated for the matrices in Appendix C. If this criterion should not be met for some matrix, A, the authors would like to know about it. For computational convenience we

computed $\frac{\|A\| - \|U\Sigma V^T\|}{\|A\|}$ for the test matrices.

Robustness of this mathematical software is established to the extent of exposing test matrices on which the algorithm has performed correctly.

Professor Gene Golub suggested two additional tests. These are

- 1) Decompose A to give $U\Sigma V^T$. Permute σ_i , reform $A=U\Sigma V^T$, and recompute the decomposition. This gives the effect of a perturbation on A in the sense that the resulting decomposition will show a permutation of the columns of U and V, yet give the same singular values of A. As additional tests we have taken orthogonal matrices U and V, particular σ_i , formed $U(\Sigma V^T)=A$ and computed $A=U\Sigma V^T$. Denote the maximum singular value by σ_{\max} and the minimum singular value by σ_{\min} . If $\frac{\sigma_{\min}}{\sigma_{\max}}$ is

less than the relative machine precision, the computed σ_{\min} may not be less than the relative precision of the machine on which it is computed, i.e. 2^{-52} for long

precision, 2^{-20} for short precision, on the IBM 360/370 machines.

- 2) Calculate the residuals $r = Ax - b$ to observe the error between the true solution x and the computed solution \hat{x} .

From Golub's formulation

$$\frac{\|x - \hat{x}\|}{\|x\|} \leq \epsilon \kappa(A) + \epsilon \kappa^2(A) \frac{\|r\|}{\|\hat{x}\|}$$

in which the condition number $\kappa(A) = \frac{\sigma_{\max}}{\sigma_{\min}}$.

The second term on the right-hand side is dominant for least squares problems. In seeking the candidate solution \hat{x}_k of least norm we compute

$$\mu_k = \kappa^2(A_k) \frac{\|r_k\|}{\|\hat{x}_k\|}$$

for different choices of k . We could compute μ_k directly by forming \hat{x}_k and r_k . However, taking advantage of $\|U\| = \|V\| = 1$ it follows that

$$\mu_k = \left(\frac{\sigma_1}{\sigma_k} \right)^2 \frac{\left(\begin{matrix} m & 2 \\ \Sigma & c_i \\ i=k+1 & \end{matrix} \right)^{1/2}}{\left(\begin{matrix} k & 2 \\ \Sigma & c_i \\ i=1 & \sigma_i \end{matrix} \right)^{1/2}}$$

where $c = U^T b$. This formulation permits the appropriate choice of the best approximating matrix $A_r = U \Sigma_r V^T$ from the minimum μ_r without explicitly computing the candidate solutions \hat{x}_k . The best approximate solution is obtained when μ_k is minimum.

Frequently the question is raised about using iterative methods for computing the singular value decomposition. There is an excellent discussion of such issues in [8] along with suggestions for constructing matrices with exact singular values.

Informally, we suggest certain guidelines for using MINFIT. Whenever possible one should avoid forming the product of a matrix by its transpose. Note that the eigenvalues λ and eigenvectors X for the real symmetric matrix eigenproblem

$$AX = X\lambda$$

are immediately available from MINFIT without ever forming $A^T A$. However, if the original problem is to obtain the eigensystem of a real symmetric positive definite, negative definite, or indefinite

This matrix is extremely ill-conditioned with respect to the solution of a linear system of equations. Its smallest singular value is approximately 10^{-22} despite the fact that its smallest eigenvalue is .501. This matrix also shows that computation of the smallest eigenvalue is limited by the relative finite precision of the machine on which it is computed. That is to say, the small singular value, 10^{-22} will appear computationally to be no smaller than the order of machine precision. This result is not attributable to the construction of the algorithm, but rather to the finite precision of the machine's arithmetic.

We suggest everywhere the use of long precision on the IBM 360/370 machines to compute the solutions of linear systems of equations, eigen-systems, and the singular value decomposition. Even so, we urge extreme caution wherever the number of rows, m , or the number of columns, n , of a matrix is of more than modest size, say 200, if the matrix is dense. The quantity
$$\frac{\|A - U(\Sigma V^T)\|}{\|A\| \cdot \max(m, n)}$$
 should be the order of machine precision.

However, the computational algorithms are, in general, $O(n^3)$ or $O(mn^2)$ processes. We advise a rigorous analysis of the structure of a matrix of high dimensions before any of the numerical algebra algorithms are used. See Appendix C for some timing results on random matrices.

The singular values of a matrix can be substantially altered by scaling the original data matrix as is shown by the examples in Appendix C. Deliberately, MINFIT does not include scaling of the rows or columns of the matrix A or right-hand sides b . For the best performance of the algorithm we suggest that columns of A be equilibrated such that the sums of their elements be as nearly equal as possible. Exact powers of

16 for the 360/370 machines should be used for scaling factors so that the data is not perturbed in trailing digits. Row scaling will have the effect of introducing weights on the data in a least squares problem and therefore should be done at a user's discretion. An excellent discussion of scaling is in [6].

Lawson further points out in [6] that it is important to take advantage of information about the certainty of data. For example, if data is known to have uncertainty in the third decimal place, that digit and all that follow are arbitrary. The matrix

$$\begin{bmatrix} 1.02 & 1.09 \\ 1.05 & 1.01 \end{bmatrix}$$

if uncertain in the third figure could lead to

$$\begin{bmatrix} 1.00 & 1.00 \\ 1.00 & 1.00 \end{bmatrix} .$$

The eigenvectors of a symmetric matrix, and therefore, the singular vectors U and V from MINFIT are known only to within a constant multiplier of modulus 1. If anyone should attempt to recompute the results in Appendix C on a machine whose arithmetic is different from that of the IBM 360/67 he may observe a change in sign on the columns of U or V.

The Fortran IV subroutine MINFIT, imbedded in TROLL (see [7]), that forms the singular value decomposition and obtains a best approximate solution vector x is an adaptation of ANLF233S from the Argonne National Laboratory. ANLF233S written by Burton Garbow, ANL, is a Fortran IV translation, with certain modifications, of the Algol 60 procedure MINFIT [3]. We have augmented

ANLF233S by adding comments and producing the numerically best approximate solution x based on a particular rank tolerance chosen for the IBM 360/370 long precision arithmetic. The machine epsilon, that is, the smallest number, $\epsilon > 0$, for which $1 + \epsilon > 1$ is the floating point representation of $16^{-13} = 2^{-52}$ for the IBM 360/370 machines. The comments and the Fortran IV listing of the subroutine used at the Center is given in Appendix A. The description of the parameters for the TROLL interface is given in Appendix B. Appendix C contains selected matrices, computed solutions, and residual norm checks obtained from driver programs that use the singular value decomposition. These results were computed on the IBM 360/67. Comments, questions, or criticisms of this subroutine should be brought to the attention of the authors of this working paper.

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APPENDIX A: Listing of the Fortran IV Program MINFIT

```
C
SUBROUTINE MINFIT(NM,M,N,A,W,IP,B,IERR,RV1,RETX)
C
C   INTEGER I,J,K,L,M,N,II,IP,I1,KK,K1,LL,L1,M1,NM,ITS,IERR
C   REAL*8 A(NM,N),W(N),B(NM,IP),RV1(N)
C   REAL*8 C,F,G,H,S,X,Y,Z,EPS,SCALE,MACHEP,RKTOL
C   REAL*8 DSQRT,DMAX1,DABS,DSIGN
C   LOGICAL RETX
C
C   THIS SUBROUTINE DETERMINES, TOWARDS THE SOLUTION OF THE LINEAR
C   SYSTEM  $AX=B$ , THE SINGULAR VALUE DECOMPOSITION  $A=USV^T$  OF A REAL
C   M BY N RECTANGULAR MATRIX, FORMING U B REATHER THAN U. HOUSEHOLDER
C   BIDIAGONALIZATION AND A VARIANT OF THE QR ALGORITHM ARE USED.
C   THIS SUBROUTINE COMPUTES A CANDIDATE SOLUTION X WHEN THE
C   LOGICAL INPUT PARAMETER RETX IS SET .TRUE. THIS CANDIDATE
C   SOLUTION IS BASED ON THE RANK TOLERANCE SET TO
C   2.0D0**(-26), THE SQUARE ROOT OF THE MACHINE PRECISION
C   2.0D0**(-52).
C
C   ON INPUT:
C
C   NM MUST BE SET TO THE ROW DIMENSION OF THE TWO-DIMENSIONAL
C   ARRAY PARAMETERS AS DECLARED IN THE CALLING PROGRAM
C   DIMENSION STATEMENT. NOTE THAT NM MUST BE AT LEAST
C   AS LARGE AS THE MAXIMUM OF M AND N;
C
C   M IS THE NUMBER OF ROWS OF A AND B;
C
C   N IS THE NUMBER OF COLUMNS OF A AND THE ORDER OF V;
C
C   A CONTAINS THE RECTANGULAR COEFFICIENT MATRIX OF THE SYSTEM;
C
C   IP IS THE NUMBER OF COLUMNS OF B. IP CAN BE ZERO;
C
C   B CONTAINS THE CONSTANT COLUMN MATRIX OF THE SYSTEM
C   IF IP IS NOT ZERO. OTHERWISE B IS NOT REFERENCED.
C
C   RETX MUST BE SET .TRUE. IF THE CANDIDATE SOLUTION X IS TO
C   BE COMPUTED. IF ONLY THE SINGULAR VALUE DECOMPOSITION IS
C   DESIRED, SET RETX .FALSE.
C
C   ON OUTPUT:
C
C   A HAS BEEN OVERWRITTEN BY THE MATRIX V (ORTHOGONAL) OF THE
C   DECOMPOSITION IN ITS FIRST N ROWS AND COLUMNS. IF AN
C   ERROR EXIT IS MADE, THE COLUMNS OF V CORRESPONDING TO
C   INDICES OF CORRECT SINGULAR VALUES SHOULD BE CORRECT;
C
C   W CONTAINS THE N (NON-NEGATIVE) SINGULAR VALUES OF A (THE
C   DIAGONAL ELEMENTS OF S). THEY ARE UNORDERED. IF AN
C   ERROR EXIT IS MADE, THE SINGULAR VALUES SHOULD BE CORRECT
C   FOR INDICES IERR+1,IERR+2,...,N;
C
```

```
C
C
C           T
C   B HAS BEEN OVERWRITTEN BY U B. IF AN ERROR EXIT IS MADE,
C           T
C   THE ROWS OF U B CORRESPONDING TO INDICES OF CORRECT
C   SINGULAR VALUES SHOULD BE CORRECT;
C
C   IF RETX IS TRUE, W WILL CONTAIN THE DIAGONAL OF THE PSEUDOINVERSE
C   OF THE DIAGONAL MATRIX S. ANY SINGULAR VALUES THAT
C   ARE LESS THAN RKTOL TIMES THE LARGEST SINGULAR VALUE ARE
C   SET TO ZERO IN THE PSEUDOINVERSE.
C
C           T
C   ALSO, THE SOLUTION X IS RETURNED IN B, REPLACING U B.
C
C   IERR IS SET TO
C   ZERO   FOR NORMAL RETURN,
C   K      IF THE K-TH SINGULAR VALUE HAS NOT BEEN
C          DETERMINED AFTER 30 ITERATIONS,
C   -1     IF THE MAXIMUM SINGULAR VALUE IS ZERO (INDICATING
C          A ZERO MATRIX ON INPUT). ONLY SET IF
C          RETX IS .TRUE..
C
C   RV1 IS A TEMPORARY STORAGE ARRAY.
C
C-----
C
C   :::::::::::  MACHEP IS A MACHINE DEPENDENT PARAMETER SPECIFYING
C               THE RELATIVE PRECISION OF FLOATING POINT ARITHMETIC
C               MACHEP = 16.000**(-13) FOR LONG FORM ARITHMETIC
C               ON S360 :::::::::::
C   DATA MACHEP/Z3410000000000000/
C   :::::::::::  RKTOL, FOR THESE APPLICATIONS, IS THE SQUARE
C               ROOT OF MACHEP :::::::::::
C   DATA RKTOL/Z3A40000000000000/
C   :::::::::::  HOUSEHOLDER REDUCTION TO BIDIAGONAL FORM :::::::::::
C   IERR = 0
C   G = 0.000
C   SCALE = 0.000
C   X = 0.000
C
C   DO 300 I = 1, N
C       L = I + 1
C       RV1(I) = SCALE * G
C       G = 0.000
C       S = 0.000
C       SCALE = 0.000
C       IF (I .GT. M) GO TO 210
C
C   DO 120 K = I, M
120  SCALE = SCALE + DABS(A(K,I))
C
C       IF (SCALE .EQ. 0.000) GO TO 210
C
C   DO 130 K = I, M
C       A(K,I) = A(K,I) / SCALE
C       S = S + A(K,I)**2
```

```
130 CONTINUE
C
  F = A(I,I)
  G = -DSIGN(DSQRT(S),F)
  H = F * G - S
  A(I,I) = F - G
  IF (I .EQ. N) GO TO 160
C
  DO 150 J = L, N
    S = 0.000
C
    DO 140 K = I, M
      140 S = S + A(K,I) * A(K,J)
C
      F = S / H
C
      DO 150 K = I, M
        A(K,J) = A(K,J) + F * A(K,I)
  150 CONTINUE
C
  160 IF (IP .EQ. 0) GO TO 190
C
  DO 180 J = 1,IP
    S = 0.000
C
    DO 170 K = I, M
      170 S = S + A(K,I) * B(K,J)
C
      F = S / H
C
      DO 180 K = I, M
        B(K,J) = B(K,J) + F * A(K,I)
  180 CONTINUE
C
  190 DO 200 K = I, M
    200 A(K,I) = SCALE * A(K,I)
C
  210 W(I) = SCALE * G
    G = 0.000
    S = 0.000
    SCALE = 0.000
    IF (I .GT. M .OR. I .EQ. N) GO TO 290
C
    DO 220 K = L, N
      220 SCALE = SCALE + DABS(A(I,K))
C
    IF (SCALE .EQ. 0.000) GO TO 290
C
    DO 230 K = L, N
      A(I,K) = A(I,K) / SCALE
      S = S + A(I,K)**2
  230 CONTINUE
C
  F = A(I,L)
  G = -DSIGN(DSQRT(S),F)
```

```
      H = F * G - S
      A(I,L) = F - G
C
      DO 240 K = L, N
240     RV1(K) = A(I,K) / H
C
      IF (I .EQ. M) GO TO 270
C
      DO 260 J = L, M
        S = 0.000
C
        DO 250 K = L, N
250         S = S + A(J,K) * A(I,K)
C
        DO 260 K = L, N
          A(J,K) = A(J,K) + S * RV1(K)
260     CONTINUE
C
270     DO 280 K = L, N
280     A(I,K) = SCALE * A(I,K)
C
290     X = DMAX1(X,DABS(W(I))+DABS(RV1(I)))
300 CONTINUE
C
      ::::::::::: ACCUMULATION OF RIGHT-HAND TRANSFORMATIONS :::::::::::
C
      ::::::::::: FOR I=N STEP -1 UNTIL 1 DO -- :::::::::::
      DO 400 II = 1, N
        I = N + 1 - II
        IF (I .EQ. N) GO TO 390
        IF (G .EQ. 0.000) GO TO 360
        H = A(I,L) * G
C
        DO 320 J = L, N
320         A(J,I) = A(I,J) / H
C
        DO 350 J = L, N
          S = 0.000
C
          DO 340 K = L, N
340           S = S + A(I,K) * A(K,J)
C
          DO 350 K = L, N
            A(K,J) = A(K,J) + S * A(K,I)
350         CONTINUE
C
360         DO 380 J = L, N
          A(I,J) = 0.000
          A(J,I) = 0.000
380         CONTINUE
C
390         A(I,I) = 1.000
          G = RV1(I)
          L = I
400 CONTINUE
C
      IF (M .GE. N .OR. IP .EQ. 0) GO TO 510
```

```
      M1 = M + 1
C
      DO 500 I = M1, N
C
          DO 500 J = 1, IP
              B(I,J) = 0.000
500 CONTINUE
C      ::::::::::: DIAGONALIZATION OF THE BIDIAGONAL FORM :::::::::::
510 EPS = MACHEP * X
C      ::::::::::: FOR K=N STEP -1 UNTIL 1 DO -- :::::::::::
      DO 700 KK = 1, N
          K1 = N - KK
          K = K1 + 1
          ITS = 0
C      ::::::::::: TEST FOR SPLITTING.
C      FOR L=K STEP -1 UNTIL 1 DO -- :::::::::::
520      DO 530 LL = 1, K
          L1 = K - LL
          L = L1 + 1
          IF (DABS(RV1(L)) .LE. EPS) GO TO 565
C      ::::::::::: RV1(1) IS ALWAYS ZERO, SO THERE IS NO EXIT
C      THROUGH THE BOTTOM OF THE LOOP :::::::::::
          IF (DABS(W(L1)) .LE. EPS) GO TO 540
530      CONTINUE
C      ::::::::::: CANCELLATION OF RV1(L) IF L GREATER THAN 1 :::::::::::
540      C = 0.000
          S = 1.000
C
          DO 560 I = L, K
              F = S * RV1(I)
              RV1(I) = C * RV1(I)
              IF (DABS(F) .LE. EPS) GO TO 565
              G = W(I)
              H = DSQRT(F*F+G*G)
              W(I) = H
              C = G / H
              S = -F / H
              IF (IP .EQ. 0) GO TO 560
C
          DO 550 J = 1, IP
              Y = B(L1,J)
              Z = B(I,J)
              B(L1,J) = Y * C + Z * S
              B(I,J) = -Y * S + Z * C
550      CONTINUE
C
560      CONTINUE
C      ::::::::::: TEST FOR CONVERGENCE :::::::::::
565      Z = W(K)
          IF (L .EQ. K) GO TO 650
C      ::::::::::: SHIFT FROM BOTTOM 2 BY 2 MINOR :::::::::::
          IF (ITS .EQ. 30) GO TO 1000
          ITS = ITS + 1
          X = W(L)
          Y = W(K1)
```

```
G = RV1(K1)
H = RV1(K)
F = ((Y - Z) * (Y + Z) + (G - H) * (G + H)) / (2.000 * H * Y)
G = DSQRT(F*F+1.000)
F = ((X - Z) * (X + Z) + H * (Y / (F + DSIGN(G,F)) - H)) / X
C ::::::::::: NEXT QR TRANSFORMATIUN :::::::::::
C   C = 1.000
C   S = 1.000

DO 600 I1 = L, K1
  I = I1 + 1
  G = RV1(I)
  Y = W(I)
  H = S * G
  G = C * G
  Z = DSQRT(F*F+H*H)
  RV1(I1) = Z
  C = F / Z
  S = H / Z
  F = X * C + G * S
  G = -X * S + G * C
  H = Y * S
  Y = Y * C

DO 570 J = 1, N
  X = A(J,I1)
  Z = A(J,I)
  A(J,I1) = X * C + Z * S
  A(J,I) = -X * S + Z * C
570 CONTINUE

Z = DSQRT(F*F+H*H)
W(I1) = Z
C ::::::::::: ROTATION CAN BE ARBITRARY IF Z IS ZERO :::::::::::
IF (Z .EQ. 0.000) GO TO 580
C   C = F / Z
C   S = H / Z
580 F = C * G + S * Y
X = -S * G + C * Y
IF (IP .EQ. 0) GO TO 600

DO 590 J = 1, IP
  Y = B(I1,J)
  Z = B(I,J)
  B(I1,J) = Y * C + Z * S
  B(I,J) = -Y * S + Z * C
590 CONTINUE

600 CONTINUE

RV1(L) = 0.000
RV1(K) = F
W(K) = X
GO TO 520
C ::::::::::: CONVERGENCE :::::::::::
```



```
650   IF (Z .GE. 0.000) GO TO 700
C     ::::::::::: W(K) IS MADE NON-NEGATIVE :::::::::::
      W(K) = -Z
C
      DO 690 J = 1, N
690   A(J,K) = -A(J,K)
C
700  CONTINUE
      IF (.NOT. RETX) GO TO 1001
C     ::::::::::: FIND MAXIMUM ELEMENT OF W :::::::::::
      Z = 0.000
      DO 750 J = 1, N
        X = W(J)
        IF (X .LE. Z) GO TO 750
        Z = X
750  CONTINUE
      IF (Z .EQ. 0) GO TO 999
C     ::::::::::: FORM PSEUDO INVERSE OF DIAG(W) :::::::::::
      DO 800 J = 1, N
        X = W(J) / Z
        IF (X .LE. RKTOL) GO TO 790
        W(J) = 1.000 / W(J)
        GO TO 800
790   W(J) = 0.000
800  CONTINUE
C     ::::::::::: FORM X (RETURNED IN B) :::::::::::
      DO 900 J = 1, IP
C
      DO 810 I = 1, N
        RV1(I) = W(I) * B(I,J)
810  CONTINUE
C
      DO 890 I = 1, N
C
        X = 0.000
        DO 850 I1 = 1, N
          X = X + A(I,I1) * RV1(I1)
850  CONTINUE
C
        B(I,J) = X
C
890  CONTINUE
C
900  CONTINUE
C
      GO TO 1001
C     ::::::::::: ERROR IF MAX SINGULAR VALUE = 0 :::::::::::
999  K=-1
C     ::::::::::: SET ERROR -- NO CONVERGENCE TO A
C           SINGULAR VALUE AFTER 30 ITERATIONS :::::::::::
1000 IERR = K
1001 RETURN
C     ::::::::::: LAST CARD OF MINFIT :::::::::::
      END
```

APPENDIX B: TROLL Implementation of MINFIT and Associated Output

The calling sequence for using the singular value decomposition within the TROLL environment is considerably different than that for the Fortran subroutine listed in Appendix A. This is a consequence of the basic design features of TROLL. However all computations are actually performed by the routine listed in Appendix A.

The TROLL version of the singular value decomposition is a function named MINFIT. Since it is a function, it returns a single data file as its result, and by TROLL convention it may not modify any of its arguments.

The format of the TROLL call to MINFIT is

$$result = \text{MINFIT} (A\text{-matrix} \langle, B\text{-matrix} \langle, code \rangle \rangle)$$

where the $\langle \rangle$ indicate optional arguments.

Since we may desire several matrices as output from MINFIT, the data file returned as *result* may be made up of several matrices. The precise result returned by MINFIT is controlled by the *code* parameter as described in the following table for the linear system:

$$\begin{array}{c}
 A \quad X = B \\
 m \times n \quad n \times p
 \end{array}
 \quad
 \begin{array}{l}
 \text{where } A = U \Sigma V^T \\
 \text{and } W = \text{diagonal of } \Sigma
 \end{array}$$

<i>Code</i>	<i>B-matrix omitted</i>	<i>B-matrix present</i>
0	illegal	X (n x p) (default)
1	V (n x n) (default)	V (n x n)
2	W (n x 1)	W (n x 1)
3	illegal	$U^T B$ (n x p)
4	$ \begin{bmatrix} W \\ V \end{bmatrix} \begin{pmatrix} 1 \times n \\ n \times n \end{pmatrix} $	$ \begin{bmatrix} W \\ V \\ (U^T B)^T \end{bmatrix} \begin{pmatrix} 1 \times n \\ n \times n \\ p \times n \end{pmatrix} $

The correspondence between the TROLL parameters and the Fortran parameters is as follows:

Immediately prior to TROLL call to Fortran routine

<u>TROLL</u>	<u>Fortran parameter</u>
Max (number of rows of <i>A-matrix</i> , number of columns <i>A-matrix</i>)	NM
Number of rows of <i>A-matrix</i>	M
Number of columns of <i>A-matrix</i>	N
<i>A-matrix</i>	A
free storage	W
if <i>B-matrix</i> omitted then 0 else number of columns of <i>B-matrix</i>	IP
not set	IERR
free storage	RV1
if <i>code</i> = 0 or <i>code</i> omitted and <i>B-matrix</i> is present then .TRUE. else .FALSE.	RETX

After call of Fortran routine

If IERR is not zero then print appropriate error message, otherwise

<u>Code</u>	<u>Fortran variable to be used as result</u>
0	B (the solution X is formed in B)
1	A
2	W
3	B
4	$\begin{bmatrix} W \\ A \end{bmatrix} \begin{matrix} \text{lxn} \\ \text{nxm} \end{matrix} \text{ or if } B\text{-matrix was specific } \begin{bmatrix} W \\ A \\ B \end{bmatrix} \begin{matrix} \text{lxn} \\ \text{nxn} \\ \text{nxp} \end{matrix}$

For more details on the use of the TROLL function, see [7].

The following output is the result of performing the TROLL version of MINFIT on the Longley data described in Appendix C. Row 1 of the matrix contains W, rows 2 through 8 contain the V matrix, and row 9 is $(U^T b)^T$.

MINFIT(LONGLEY_X, LONGLEY_Y, 4)

ROW	COLUMN 1	COLUMN 2	COLUMN 3	COLUMN 4	COLUMN 5	COLUMN 6	COLUMN 7
1	1.6637E+06	8.3900E+04	3.4057E+03	1.5848E+03	41.654200	3.4323E-04	3.6504E+00
2	-2.3417E-06	1.0798E-05	-9.7316E-06	2.8160E-06	-5.1038E-04	-1.0000E+00	3.4181E-05
3	-2.4376E-04	6.1669E-04	-4.9654E-04	-1.4370E-03	-1.0442E-01	1.9307E-05	-9.9453E-01
4	-9.6034E-01	-2.7878E-01	-2.2179E-03	4.6324E-03	-1.3505E-03	-3.0688E-08	1.9871E-04
5	-7.7734E-03	1.0335E-02	7.8544E-01	-6.1856E-01	-1.7084E-02	-4.5778E-07	2.3034E-03
6	-6.2675E-03	1.3422E-02	-6.1866E-01	-7.8548E-01	8.0722E-03	-1.3094E-07	6.0617E-04
7	-2.7861E-01	9.5998E-01	-4.8046E-05	1.8883E-02	2.1381E-02	1.0430E-07	-1.6086E-03
8	-4.5794E-03	2.0892E-02	-1.8467E-02	4.8026E-03	-9.9412E-01	5.1138E-04	1.0439E-01
9	-2.5750E+05	4.6093E+04	-2.8832E+03	1.6039E+03	-1.7736E+03	1.1890E+03	210.980000

APPENDIX C: Selected Matrices, Computed Solutions, and Illustrative Examples

This appendix displays a representative sample of matrices on which the subroutine MINFIT has performed satisfactorily. The input matrices and the output computations have been retained on magnetic tape. The format of the printing was chosen for convenience and does not include the full fifteen decimal place output that was produced by the long precision computation on the machine. If anyone should attempt to reproduce these results on a machine whose arithmetic or relative precision is different from that of the IBM 360/67 he may get output that is different from that which we display. However, such results should be correct to the order of machine precision on which the computation is performed.

Though we include certain matrices of the Hilbert segments, we do not encourage their use as test matrices for software validation. The Hilbert segments are not representable exactly in a computing machine unless appropriate multipliers are used to preclude a perturbation on input of the data. We have used such multipliers.

Other matrices exhibited are a 3x3 matrix that is contrived to display information about near dependencies of rows or columns, a test matrix from [1]^{*} and [2] and a matrix suggested by Ed Kuh. The matrix from [1] is exactly representable in the machine though it is ill conditioned with respect to the solution of linear systems of equations. The matrix in [3] shows the dependence of the solution vector x on the rank tolerance that is chosen.

On the output that is displayed, V has its usual meaning, W contains the unordered singular values from MINFIT, P is an integer vector that indicates the descending order of the singular values, MU contains μ_i for $i=1,2,\dots,n$ for each right-hand side and C contains $U^T b$. X contains the candidate solution of $Ax=b$. $IERR$ is the error indicator from MINFIT; it is non-zero if the computation of any singular value requires more than 30 iterations or if the maximum singular value is zero.

^{*}Numerals in square brackets refer to entries in the Reference section, p. C14.

This 3x3 matrix shows output that indicates rank 2 if the smallest singular value is treated as zero. Given this interpretation, columns 1 and 2 are linearly dependent. This information is contained in column 2 of the V matrix.

```
A=
( ROW 1 ):
0.10101000 01 0.10098000 01 0.98000000 00
( ROW 2 ):
0.10098000 01 0.10104000 01 0.98000000 00
( ROW 3 ):
0.98000000 00 0.98000000 00 0.10100000 01
```

```
H=
(COLUMN 1)
0.10000000 01 0.0 0.0
(COLUMN 2)
0.0 0.10000000 01 0.0
(COLUMN 3)
0.0 0.0 0.10000000 01
```

IERR = 0

```
V =
(COLUMN 1)
-0.57927490 00 -0.57933300 00 -0.57342300 00
(COLUMN 2)
-0.70801190 00 0.70619830 00 0.17604610-02
(COLUMN 3)
-0.40393050 00 -0.40701010 00 0.81925760 00
```

```
W=
0.29901010 01 0.44980760-03 0.39948830-01
```

```
C=
(COLUMN 1)
-0.57927490 00 -0.70801190 00 -0.40393050 00
(COLUMN 2)
-0.57933300 00 0.70619830 00 -0.40701010 00
(COLUMN 3)
-0.57342300 00 0.17604610-02 0.81925760 00
```

P = 1 3 2

```
MU=
(COLUMN 1)
0.46150140 02 0.88407600 00 0.56800110-02
(COLUMN 2)
0.46145510 02 0.87738910 00 0.56945950-02
(COLUMN 3)
0.46621110 02 0.43594980 00 0.42822180 00
```

```
USING MACHEP, X=
(COLUMN 1)
0.11186300 04 -0.11073520 04 -0.10943610 02
(COLUMN 2)
-0.11073520 04 0.11129910 04 -0.54718030 01
(COLUMN 3)
-0.10943610 02 -0.54718030 01 0.16917920 02
```

```
USING RK4UL, X=
(COLUMN 1)
0.11186300 04 -0.11073520 04 -0.10943610 02
(COLUMN 2)
-0.11073520 04 0.11129910 04 -0.54718030 01
(COLUMN 3)
-0.10943610 02 -0.54718030 01 0.16917920 02
```

The matrix whose data is displayed on the following page was suggested by Ed Kuh. The matrix is 32x10 and has singular values, to 4 decimal places,

4921, 41.89, 30.33, 18.71, 8.573, 2.491,
4.763, 5.532, 6.162, 6.091.

The indicated rank determination is that the matrix is of rank 10 if the data is certain in all digits, of rank 1 if the third digit is doubtful.

The residual checks for the decomposition are

MAX-ROW-SUM RESIDUAL = 0.1818241327D-14
EUCLIDIAN RESIDUAL = 0.2402697593D-14
MAX-COL-SUM RESIDUAL = 0.1378022275D-14

Truncation of the data to integers 234,231,...,311 gives singular values to 4 decimal places.

4911, 41.10, 30.07, 18.59, 8.356, 3.403,
6.299, 5.727, 4.963, 5.198

Data for A

346.6	Row 32
342.1	Row 31
337.9	Row 30
337.9	
331.2	
326.7	
321.8	
314.5	
312.2	
311.7	
311.6	
307.4	
303.8	
300.8	
294.6	
290.7	
286.4	
283.2	
278.9	
272.6	
266.2	
262.4	
257.3	
254.7	
255.3	
254.0	
253.8	
253.4	
249.2	
245.8	
240.9	
234.4	Row 1
231.7	
231.2	
227.9	
226.0	
220.8	
214.7	
209.0	
201.5	
202.2	

Right-hand side B

214.6
216.7
225.0
228.4
230.1
231.0
230.3
232.3
234.6
237.3
241.8
247.7
252.7
256.8
260.4
262.0
264.4
267.5
272.8
277.2
279.3
283.8
285.4
284.5
287.4
292.2
296.2
304.0
309.8
314.8
316.3
321.1

The Hilbert matrix of order 7, generated in long precision, 7 digits of which are given for each element, is inexact in the machine.

```
A=
( ROW 1 ):
0.1000000D 01 0.5000000D 00 0.3333333D 00 0.2500000D 00 0.2000000D 00 0.1666667D 00 0.1428571D 00
( ROW 2 ):
0.5000000D 00 0.3333333D 00 0.2500000D 00 0.2000000D 00 0.1666667D 00 0.1428571D 00 0.1250000D 00
( ROW 3 ):
0.3333333D 00 0.2500000D 00 0.2000000D 00 0.1666667D 00 0.1428571D 00 0.1250000D 00 0.1111111D 00
( ROW 4 ):
0.2500000D 00 0.2000000D 00 0.1666667D 00 0.1428571D 00 0.1250000D 00 0.1111111D 00 0.1000000D 00
( ROW 5 ):
0.2000000D 00 0.1666667D 00 0.1428571D 00 0.1250000D 00 0.1111111D 00 0.1000000D 00 0.9090909D-01
( ROW 6 ):
0.1666667D 00 0.1428571D 00 0.1250000D 00 0.1111111D 00 0.1000000D 00 0.9090909D-01 0.8333333D-01
( ROW 7 ):
0.1428571D 00 0.1250000D 00 0.1111111D 00 0.1000000D 00 0.9090909D-01 0.8333333D-01 0.7692308D-01
```

Its singular values are

```
W=
0.1660885D 01 0.2719202D 00 0.2128975D-01 0.1008588D-02 0.2938637D-04 0.4856763D-06 0.3493744D-08
```

Multiplication of the Hilbert matrix of order 7 by the constant
360360 allows a machine representation that is exact.

```
A=
( ROW 1 ):
0.36036000 06 0.18018000 06 0.12012000 06 0.90090000 05 0.72072000 05 0.60060000 05 0.51480000 05
( ROW 2 ):
0.18018000 06 0.12012000 06 0.90090000 05 0.72072000 05 0.60060000 05 0.51480000 05 0.45045000 05
( ROW 3 ):
0.12012000 06 0.90090000 05 0.72072000 05 0.60060000 05 0.51480000 05 0.45045000 05 0.40040000 05
( ROW 4 ):
0.90090000 05 0.72072000 05 0.60060000 05 0.51480000 05 0.45045000 05 0.40040000 05 0.36036000 05
( ROW 5 ):
0.72072000 05 0.60060000 05 0.51480000 05 0.45045000 05 0.40040000 05 0.36036000 05 0.32760000 05
( ROW 6 ):
0.60060000 05 0.51480000 05 0.45045000 05 0.40040000 05 0.36036000 05 0.32760000 05 0.30030000 05
( ROW 7 ):
0.51480000 05 0.45045000 05 0.40040000 05 0.36036000 05 0.32760000 05 0.30030000 05 0.27720000 05
```

Its singular values are

```
W=
0.59851660 06 0.97989160 05 0.76719760 04 0.36345460 03 0.10589670 02 0.17501830 00 0.12590610-02
```

The Longley data matrix [3] with its associated output is

```
A =
( ROW 1 ):
0.10000000 01 0.83000000 02 0.23428900 06 0.23560000 04 0.15900000 04 0.10760800 06 0.19470000 04
( ROW 2 ):
0.10000000 01 0.88500000 02 0.25942600 06 0.23250000 04 0.14560000 04 0.10863200 06 0.19480000 04
( ROW 3 ):
0.10000000 01 0.88200000 02 0.25805400 06 0.36870000 04 0.16160000 04 0.10977300 06 0.19490000 04
( ROW 4 ):
0.10000000 01 0.89500000 02 0.28459900 06 0.33510000 04 0.16500000 04 0.11092900 06 0.19500000 04
( ROW 5 ):
0.10000000 01 0.96200000 02 0.32897500 06 0.20990000 04 0.30990000 04 0.11207500 06 0.19510000 04
( ROW 6 ):
0.10000000 01 0.98100000 02 0.34699900 06 0.19320000 04 0.35940000 04 0.11327000 06 0.19520000 04
( ROW 7 ):
0.10000000 01 0.99000000 02 0.36538500 06 0.18700000 04 0.35470000 04 0.11509400 06 0.19530000 04
( ROW 8 ):
0.10000000 01 0.10000000 03 0.36311200 06 0.35780000 04 0.33500000 04 0.11621900 06 0.19540000 04
( ROW 9 ):
0.10000000 01 0.10120000 03 0.39746900 06 0.29040000 04 0.30480000 04 0.11738800 06 0.19550000 04
( ROW 10 ):
0.10000000 01 0.10460000 03 0.41918000 06 0.28220000 04 0.28570000 04 0.11873400 06 0.19560000 04
( ROW 11 ):
0.10000000 01 0.10840000 03 0.44276900 06 0.29360000 04 0.27980000 04 0.12044500 06 0.19570000 04
( ROW 12 ):
0.10000000 01 0.11080000 03 0.44454600 06 0.46810000 04 0.26370000 04 0.12195000 06 0.19580000 04
( ROW 13 ):
0.10000000 01 0.11260000 03 0.48270400 06 0.38130000 04 0.25520000 04 0.12336600 06 0.19590000 04
( ROW 14 ):
0.10000000 01 0.11420000 03 0.50260100 06 0.39130000 04 0.25140000 04 0.12536800 06 0.19600000 04
( ROW 15 ):
0.10000000 01 0.11570000 03 0.51817300 06 0.48060000 04 0.25720000 04 0.12785200 06 0.19610000 04
( ROW 16 ):
0.10000000 01 0.11690000 03 0.55489400 06 0.40070000 04 0.28270000 04 0.13008100 06 0.19620000 04

B =
(COLUMN 1)
0.60323000 05 0.61122000 05 0.60171000 05 0.61187000 05 0.63221000 05 0.63639000 05 0.64989000 05
0.63761000 05 0.66019000 05 0.67857000 05 0.68169000 05 0.66513000 05 0.68655000 05 0.69564000 05
0.69331000 05 0.70551000 05

IERR = 0

V =
(COLUMN 1)
-0.23417280-05 -0.24375680-03 -0.96034010 00 -0.77733770-02 -0.62675480-02 -0.27861480 00 -0.45794090-02
(COLUMN 2)
0.10797810-04 0.61668600-03 -0.27878070 00 0.10334770-01 0.13421640-01 0.95997790 00 0.20891970-01
(COLUMN 3)
-0.97316110-05 -0.49653610-03 -0.22179310-02 0.78543940 00 -0.61865890 00 -0.48045890-04 -0.18466820-01
(COLUMN 4)
0.28160440-05 -0.14370220-02 0.46323930-02 -0.61856340 00 -0.78547830 00 0.18882820-01 0.48025910-02
(COLUMN 5)
-0.51038040-03 -0.10441850 00 -0.13504740-02 -0.17083690-01 0.80721570-02 0.21381020-01 -0.99412300 00
(COLUMN 6)
-0.99999990 00 0.19307120-04 -0.30687980-07 -0.45777720-06 -0.13094330-06 0.10429930-06 0.51137880-03
(COLUMN 7)
0.34180980-04 -0.99453210 00 0.19871480-03 0.23036080-02 0.60617260-03 -0.16085630-02 0.10439200 00

W =
0.16636680 07 0.83899620 05 0.34056740 04 0.15847880 04 0.41654200 02 0.34322890-03 0.36503800 01

C =
(COLUMN 1)
-0.15328510 00 0.45378580 00 0.89857260-01 0.26517570 00 0.30558470 00 0.11393900-01 0.15302070 00
-0.48465290-01 -0.40209480-02 -0.19433730 00 -0.34302910 00 -0.89768860-01 -0.11988820 00 -0.29862080 00
-0.29740200 00 -0.46626980 00

P = 1 2 3 4 5 7 6

MU =
(COLUMN 1)
0.19577650 20 0.33345700 18 0.66973430 17 0.10643310 17 0.24581320 15 0.42386460 14 0.54338150 11

USING MACHEP, X =
(COLUMN 1)
-0.34642690 07 0.13849520 02 -0.35278390-01 -0.20094190 01 -0.10251330 01 -0.52347820-01 0.18199480 04

USING RKTDL, X =
(COLUMN 1)
0.23724110-01 -0.53035530 02 0.71033030-01 -0.42355560 00 -0.57151010 00 -0.41366870 00 0.48394360 02
```

The Bauer matrix with its associated output is

A=
(ROW 1) :
-0.74000000 02 0.80000000 02 0.18000000 02 -0.11000000 02 -0.40000000 01 -0.80000000 01
(ROW 2) :
0.14000000 02 -0.69000000 02 0.21000000 02 0.28000000 02 0.0 0.70000000 01
(ROW 3) :
0.66000000 02 -0.72000000 02 -0.50000000 01 0.70000000 01 0.10000000 01 0.40000000 01
(ROW 4) :
-0.12000000 02 0.66000000 02 -0.30000000 02 -0.23000000 02 0.30000000 01 -0.30000000 01
(ROW 5) :
0.30000000 01 0.80000000 01 -0.70000000 01 -0.40000000 01 0.10000000 01 0.0
(ROW 6) :
0.40000000 01 -0.12000000 02 0.40000000 01 0.40000000 01 0.0 0.10000000 01

B=
(COLUMN 1)
0.51000000 02 -0.61000000 02 -0.56000000 02 0.69000000 02 0.10000000 02 -0.12000000 02
(COLUMN 2)
-0.56000000 02 0.52000000 02 0.76400000 03 0.40960000 04 -0.13276000 05 0.84210000 04
(COLUMN 3)
-0.50000000 01 -0.90000000 01 0.70800000 03 0.41650000 04 -0.13266000 05 0.84090000 04

IERR = 0

V =
(COLUMN 1)
0.53159590 00 -0.82429840 00 -0.38242860 -01 0.17949250 00 0.10576910 -01 0.64390190 -01
(COLUMN 2)
-0.62509500 00 -0.29815740 00 0.62845080 00 0.34816700 00 -0.63856900 -01 0.10491370 -01
(COLUMN 3)
0.33696200 00 0.10421750 00 0.65658480 00 -0.52381900 00 -0.23501730 00 -0.33892800 00
(COLUMN 4)
-0.40824830 00 -0.40824830 00 -0.40824830 00 -0.40824830 00 -0.40824830 00 -0.40824830 00
(COLUMN 5)
0.21539230 00 0.23251740 00 -0.70459190 -01 0.60620830 00 -0.63896270 00 -0.34469610 00
(COLUMN 6)
0.76299260 -02 -0.64905330 -02 -0.29192670 -01 0.19498870 00 0.60467950 00 -0.77161490 00

W=
0.17383930 03 0.64861870 02 0.10667160 02 0.10000000 01 0.17524770 00 0.47441820 -04

C=
(COLUMN 1)
-0.11457290 03 -0.35669610 02 -0.79211710 01 -0.40824830 00 0.89820800 00 -0.85865440 -04
(COLUMN 2)
0.37040050 -03 0.16174950 -03 -0.31773030 -01 -0.40824830 00 -0.19669080 01 -0.16264440 05
(COLUMN 3)
-0.11457260 03 -0.35669450 02 -0.79529440 01 -0.81649660 00 -0.10687000 01 -0.16264440 05

P = 1 2 3 4 5 6

MU=
(COLUMN 1)
0.55143120 07 0.42339880 07 0.32020640 07 0.30130790 07 0.69023290 06 0.65274640 06
(COLUMN 2)
0.23068100 15 0.14984950 15 0.16501570 12 0.12039250 10 0.43763960 08 0.14336980 01
(COLUMN 3)
0.74578680 09 0.57262870 09 0.43232170 09 0.35115200 09 0.78558700 08 0.14337370 01

USING MACHEP, X=
(COLUMN 1)
0.10000000 01 0.20000000 01 -0.10000000 01 0.30000000 01 -0.40000000 01 -0.12249380 -09
(COLUMN 2)
-0.26157640 07 0.22251420 07 0.10008100 08 -0.66847850 08 -0.20730180 09 0.26453220 09
(COLUMN 3)
-0.26157630 07 0.22251440 07 0.10008100 08 -0.66847850 08 -0.20730180 09 0.26453220 09

USING RKTOL, X=
(COLUMN 1)
0.10000000 01 0.20000000 01 -0.10000000 01 0.30000000 01 -0.40000000 01 -0.12249380 -09
(COLUMN 2)
-0.26157640 07 0.22251420 07 0.10008100 08 -0.66847850 08 -0.20730180 09 0.26453220 09
(COLUMN 3)
-0.26157630 07 0.22251440 07 0.10008100 08 -0.66847850 08 -0.20730180 09 0.26453220 09

The condition number of a nonsingular matrix may be improved by row or column scaling. The Bauer matrix, scaled as

```
A=
( ROW 1 ):
-0.74000000 02  0.80000000 02  0.36000000 02 -0.33000000 02 -0.40000000 02 -0.80000000 02
( ROW 2 ):
 0.14000000 02 -0.69000000 02  0.42000000 02  0.84000000 02  0.0                0.70000000 02
( ROW 3 ):
 0.66000000 02 -0.72000000 02 -0.10000000 02  0.21000000 02  0.10000000 02  0.40000000 02
( ROW 4 ):
-0.12000000 02  0.66000000 02 -0.60000000 02 -0.69000000 02  0.30000000 02 -0.30000000 02
( ROW 5 ):
 0.24000000 02  0.64000000 02 -0.11200000 03 -0.96000000 02  0.80000000 02  0.0
( ROW 6 ):
 0.28000000 02 -0.84000000 02  0.56000000 02  0.84000000 02  0.0                0.70000000 02
```

with singular values

```
W=
0.29594490 03  0.18165700 03  0.48937800 02  0.12882170 02  0.70959950 00  0.13971070-02
```

The singular value decomposition provides $U\Sigma V^T$ as the decomposition of a matrix A. Given the orthonormal columns U and V one can form another matrix $U\Sigma V^T$ for arbitrary Σ . Using U and V from the inexact Hilbert matrix of order 7, the reformed matrix

```
THE REFORMED A =
( ROW 1 ):
0.20106490 02 -0.11191230 03  0.23250410 03 -0.24893840 03  0.14774330 03 -0.46373370 02  0.60402080 01
( ROW 2 ):
-0.11191230 03  0.13209940 04 -0.47280010 04  0.78498420 04 -0.67653190 04  0.29490710 04 -0.51555810 03
( ROW 3 ):
0.23250410 03 -0.47280010 04  0.25364010 05 -0.58889480 05  0.67996620 05 -0.38558890 05  0.85824910 04
( ROW 4 ):
-0.24893840 03  0.78498420 04 -0.58889480 05  0.18005690 06 -0.26360290 06  0.18470440 06 -0.49868680 05
( ROW 5 ):
0.14774330 03 -0.67653190 04  0.67996620 05 -0.26360290 06  0.47139410 06 -0.39302090 06  0.12386200 06
( ROW 6 ):
-0.46373370 02  0.29490710 04 -0.38558890 05  0.18470440 06 -0.39302090 06  0.37926500 06 -0.13550680 06
( ROW 7 ):
0.60402080 01 -0.51555810 03  0.85824910 04 -0.49868680 05  0.12386200 06 -0.13550680 06  0.53689920 05
```

where the σ_i are 10^{-8} , 10^{-7} , 10^{-6} , 10^{-5} , 10^{-4} , 10^{-3} and 10^{-2} .

The computed σ_i from the reformed A are

```
W=
0.10000000 07  0.10000000 06  0.10000000 05  0.10000000 04  0.10000000 03  0.10000000 01  0.10000000 02
MAX-ROW-SUM RESIDUAL = 0.1228389490D-14
EUCLIDEAN RESIDUAL = 0.9990491258D-15
MAX-COL-SUM RESIDUAL = 0.1228389490D-14
```

However, choosing $\sigma_i = 10^{24}, 10^{20}, 10^{16}, 10^{12}, 10^8, 10^4, 10^0$ gives

```
W=
0.1000000D 25 0.1000000D 21 0.1000000D 17 0.2608234D 08 0.1000001D 13 0.2189502D 08 0.3546465D 07
MAX-ROW-SUM RESIDUAL = 0.6067562603D-15
EUCLIDEAN RESIDUAL = 0.4697620457D-15
MAX-COL-SUM RESIDUAL = 0.4045041735D-15
```

The singular values smaller than 10^{12} are effected by the order of machine precision relative to σ_{\max} .

Choosing $\sigma_i = 10^0, 10^{-4}, 10^{-8}, 10^{-12}, 10^{-16}, 10^{-20}, 10^{-24}$ gives

```
W=
0.1000000D 01 0.1000000D-05 0.1000000D-07 0.9999812D-12 0.1104082D-15 0.1852770D-16 0.2530714D-17
MAX-ROW-SUM RESIDUAL = 0.1316051070D-14
EUCLIDEAN RESIDUAL = 0.8881784153D-15
MAX-COL-SUM RESIDUAL = 0.2642102139D-15
```


<u>N</u>	<u>Time in seconds</u>
5	.074
10	.464
20	3.490
40	25.010
60	79.353
80	185.653

These times were obtained from the interval timer on the 67 which gives approximate microseconds at 13 microsecond intervals. These timings were obtained at the NBER Computer Research Center by Harry Bochner.

The time required by MINFIT is approximately that of SVD if U , V , and Σ are computed. However, in general, U is not needed. The time that is used to form V , Σ , and $U^T b$ is therefore reduced by almost 50% of the times listed here.

The time for computation of the singular value decomposition will be matrix dependent in that fewer iterations may be required when there are multiplicities or clusters of singular values.

References

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2. Golub, G. H. and Reinsch, C., "Singular Value Decomposition and Least Squares Solutions," in J. H. Wilkinson and C. Reinsch (eds.) Handbook for Automatic Computation, Volume II: Linear Algebra, Springer Verlag, 134-151 (1971); prepublished in Numer. Math. 14, 403-420 (1970).
3. Longley, James W., "An Appraisal of Least Squares Programs for the Electronic Computer from the Point of View of the User," JASA 62, 819-841, 1967.