

Algorithms in the Nashlib set in various programming languages

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Abstract

Algorithms from the book Nash (1979) are implemented in a variety of programming languages including Fortran, BASIC, Pascal, Python and R.

Overview of this document

A companion document **Overview of Nashlib and its Implementations** describes the process and computing environments for the implementation of Nashlib algorithms. This document gives comments and/or details relating to implementations of the algorithms themselves.

Note that some discussion of the reasoning behind certain choices in algorithms or implementations are given in the Overview document.

Algorithms 1 and 2 – one-sided SVD and least squares solution

These were two of the first algorithms to interest the first author in compact codes. At the time (1973-1978) he was working at Agriculture Canada in support of econometric modeling. More or less “regular” computers required accounts linked to official projects, but there was a time-shared Data General NOVA that offered 4K to 7K byte working spaces for data and programs in interpreted BASIC. BASIC of a very similar dialect was available also on an HP 9830 calculator. On these machines, availability of a terminal or the calculator was the only limitation to experimentation with recent innovations in algorithms. In particular, a lot of modeling was done with linear least squares regression, mostly using the traditional normal equations. The singular value decomposition and other methods such as the Householder, Givens or Gram-Schmidt approaches to the QR matrix decomposition were relatively recent innovations. However, the code for the Golub-Kahan SVD was rather long for both the hardware and the BASIC language. Instead, a one-sided Jacobi method was developed from ideas of Hestenes (1958) and Chartres (1962). Some work by Kaiser (1972) was also observed. Later workers have generally credited Hestenes with this approach, and he certainly wrote about it, but we (JN) suspect strongly that he never actually attempted an implementation. In a conversation at a conference, Chartres said that some experiments were tried, but that he believed no production usage occurred. We must remember that access to computers until the 1970s was quite difficult.

The method published in Nash (1975) and later revised in Nash and Shlien (1987) ignored some advice that Jacobi rotations should not use angles greater than $\pi/4$ (see Forsythe and Henrici (1960)). This allowed of a cyclic process that not only developed a form of the decomposition, but also sorted it to effectively present the singular values in descending order of size. This avoided extra program code of about half the length of the svd routine.

About 2 decades after Nash (1975), there was renewed interest in one-sided Jacobi methods, but rather little acknowledgment of the earlier development, and much more complicated codes. ?? How far to reference more recent developments??

Fortran

Listing

Note that this is a single precision code. Very few modern calculations are carried out at this precision. Moreover, the dialect of Fortran (Fortran 77) is now decidedly old-fashioned, though it compiles and executes just fine.

```
C&&& A1-2
C TEST ALGS. 1 & 2 J.C. NASH JULY 1978, APRIL 1989
C USES FRANK MATRIX COLUMNS
      LOGICAL ESVD,NTOL
      INTEGER N,ND,IPOS(10),NVAR,MD,I,J,K,YPOS,M
      REAL A(30,10),D(30,11),G(30),X(10),Z(10),Y(30),Q,V(10,10),EPS
      EXTERNAL FRANKM
C I/O CHANNELS
      NIN=5
      NOUT=6
      ND=10
      MD=30
      D(1,1)=5
      D(1,2)=1.0E-6
      D(1,3)=1
      Y(1)=1
      D(2,1)=6
      D(2,2)=0.999999
      D(2,3)=1
      Y(2)=2
```

```

D(3,1)=7
D(3,2)=2.00001
D(3,3)=1
Y(3)=3
D(4,1)=8
D(4,2)=2.9999
D(4,3)=1
Y(4)=4
N=3
M=4
DO 30 J=1,N
DO 25 I=1,M
    A(I,J)=D(I,J)
25 CONTINUE
30 CONTINUE
ESVD=.FALSE.
WRITE(NOUT,955)(Y(I),I=1,M)
955 FORMAT(1H ,5E16.8)
NTOL=.FALSE.
Q = 1e-5
WRITE(NOUT,956)Q
956 FORMAT(' SING. VALS. .LE.',E16.8,' ARE PRESUMED ZERO')
IF(Q.LT.0.0) STOP
C "MACHINE PRECISION" VALUE
EPS=1E-6
CALL A2LSVD(M,N,A,MD,EPS,V,ND,Z,NOUT,Y,G,X,Q,ESVD,NTOL)
WRITE(NOUT,957)(J,X(J),J=1,N)
957 FORMAT(' X(',I3,')=',1PE16.8)
STOP
END
SUBROUTINE OUT(A,NA,N,NP,NOUT)
C J.C. NASH JULY 1978, APRIL 1989
INTEGER NA,N,NOUT,I,J
REAL A(NA,NP)
DO 20 I=1,N
    WRITE(NOUT,951)I
951 FORMAT(' ROW',I3)
    WRITE(NOUT,952)(A(I,J),J=1,NP)
952 FORMAT(1H ,1PE16.8)
20 CONTINUE
RETURN
END
SUBROUTINE FRANKM(M,N,A,NA)
C J.C. NASH JULY 1978, APRIL 1989
INTEGER M,N,NA,I,J
C INPUTS FRANK MATRIX M BY N INTO A
REAL A(NA,N)
DO 20 I=1,M
    DO 10 J=1,N
        A(I,J)=AMINO(I,J)
10 CONTINUE
20 CONTINUE
RETURN

```

```

      END
      SUBROUTINE A3PREP(M,N1,A,NA,AIN)
C   PREPARE A3 TEST
C   J.C. NASH   JULY 1978, APRIL 1989
C   MATRIX M BY N=N1-1 IS INPUT VIA SUBROUTINE AIN
C   COL. N1 IS SET TO SUM OF OTHER COLS.  - UNIT SOLUTION ELEMENTS
C   BUT ONLY IF M=N - OTHERWISE SIMPLY INPUT MATRIX
C   NA = FIRST DIMENSION OF A
      INTEGER M,N1,NA,N,J,I
      REAL A(NA,N1),S
      N=N1-1
      CALL AIN(M,N,A,NA)
      IF(M.NE.N)RETURN
      DO 40 I=1,N
        S=0.0
        DO 30 J=1,N
          S=S+A(I,J)
30      CONTINUE
        A(I,N1)=S
40      CONTINUE
      RETURN
      END
      SUBROUTINE A1SVD(M,N,A,NA,EPS,V,NV,Z,IPR)
C   ALGORITHM 1 SINGULAR VALUE DECOMPOSITION BY COLUMN ORTHOGONA-
C   LISATION VIA PLANE ROTATIONS
C   J.C. NASH   JULY 1978, FEBRUARY 1980, APRIL 1989
C   M BY N MATRIX A IS DECOMPOSED TO U*Z*VT
C   A   = ARRAY CONTAINING A (INPUT), U (OUTPUT)
C   NA  = FIRST DIMENSION OF A
C   EPS = MACHINE PRECISION
C   V   = ARRAY IN WHICH ORTHOGAONAL MATRIX V IS ACCUMULATED
C   NV  = FIRST DIMENSION OF V
C   Z   = VECTOR OF SINGULAR VALUES
C   IPR = PRINT CHANNEL IF IPR.GT.0 THEN PRINTING
C   STEP 0
      INTEGER M,N,J1,N1,COUNT
      REAL A(NA,N),V(NV,N),Z(N),EPS,TOL,P,Q,R,VV,C,S
C   UNDERFLOW AVOIDANCE STRATEGY
      REAL SMALL
      SMALL=1.0E-36
C   ABOVE IS VALUE FOR IBM
      TOL=N*N*EPS*EPS
      DO 6 I=1,N
        DO 4 J=1,N
          V(I,J)=0.0
4      CONTINUE
        V(I,I)=1.0
6      CONTINUE
      N1=N-1
C   STEP 1
10     COUNT=N*(N-1)/2
C   STEP 2
      DO 140 J=1,N1

```

```

C  STEP 3
      J1=J+1
      DO 130 K=J1,N
C  STEP 4
      P=0.0
      Q=0.0
      R=0.0
C  STEP 5
      DO 55 I=1,M
        IF (ABS(A(I,J)).GT.SMALL.AND.ABS(A(I,K)).GT.SMALL)
          #      P=P+A(I,J)*A(I,K)
          IF (ABS(A(I,J)).GT.SMALL) Q=Q+A(I,J)**2
          IF (ABS(A(I,K)).GT.SMALL) R=R+A(I,K)**2
C          P=P+A(I,J)*A(I,K)
C          Q=Q+A(I,J)**2
C          R=R+A(I,K)**2
      55      CONTINUE
C  STEP 6
      IF (Q.GE.R) GOTO 70
      C=0.0
      S=1.0
      GOTO 90
C  STEP 7
      70      IF (R.LE.TOL) GOTO 120
      IF ((P*P)/(Q*R).LT.TOL) GOTO 120
C  STEP 8
      Q=Q-R
      VV=SQRT(4.0*P**2+Q**2)
      C=SQRT((VV+Q)/(2.0*VV))
      S=P/(VV*C)
C  STEP 9
      90      DO 95 I=1,M
        R=A(I,J)
        A(I,J)=R*C+A(I,K)*S
        A(I,K)=-R*S+A(I,K)*C
      95      CONTINUE
C  STEP 10
      DO 105 I=1,N
        R=V(I,J)
        V(I,J)=R*C+V(I,K)*S
        V(I,K)=-R*S+V(I,K)*C
      105     CONTINUE
C  STEP 11
      GOTO 130
      120     COUNT=COUNT-1
C  STEP 13
      130     CONTINUE
C  STEP 14
      140     CONTINUE
C  STEP 15
      IF (IPR.GT.0) WRITE (IPR,964) COUNT
      964     FORMAT(1H ,I4,10H ROTATIONS)
      IF (COUNT.GT.0) GOTO 10

```

```

C STEP 16
    DO 220 J=1,N
C STEP 17
    Q=0.0
C STEP 18
    DO 185 I=1,M
        Q=Q+A(I,J)**2
185    CONTINUE
C STEP 19
    Q=SQRT(Q)
    Z(J)=Q
    IF(IPR.GT.0)WRITE(IPR,965)J,Q
965    FORMAT( 4H SV(,I3,2H)=,1PE16.8)
C STEP 20
    IF(Q.LT.TOL)GOTO 220
C STEP 21
    DO 215 I=1,M
        A(I,J)=A(I,J)/Q
215    CONTINUE
C STEP 22
220    CONTINUE
    RETURN
    END
    SUBROUTINE A2LSVD(M,N,A,NA,EPS,V,NV,Z,IPR,Y,G,X,Q,ESVD,NTOL)
C J.C. NASH JULY 1978, FEBRUARY 1980, APRIL 1989
C SAME COMMENTS AS SUBN A1SVD EXCEPT FOR
C G = WORKING VECTOR IN N ELEMENTS
C Y = VECTOR CONTAINING M VALUES OF DEPENDENT VARIABLE
C X = SOLUTION VECTOR
C Q = TOLERANCE FOR SINGULAR VALUES. THOSE .LE. Q TAKEN AS ZERO.
C ESVD = LOGICAL FLAG SET .TRUE. IF SVD ALREADY EXISTS IN A,Z,V
C NTOL = LOGICAL FLAG SET .TRUE. IF ONLY NEW TOLERANCE Q.
    LOGICAL ESVD,NTOL
    INTEGER M,N,IPR,I,J
    REAL A(NA,N),V(NV,N),Z(N),Y(M),G(N),X(N),S,Q
C STEP 1
    IF(NTOL)GOTO 41
    IF(.NOT.ESVD)CALL A1SVD(M,N,A,NA,EPS,V,NV,Z,IPR)
    IF(IPR.GT.0)WRITE(IPR,965)(J,Z(J),J=1,N)
965    FORMAT(16H SINGULAR VALUE(,I3,2H)=,1PE16.8)
C STEP 2 VIA SUBROUTINE CALL
C ALTERNATIVE WITHOUT G
C NO STEP 3
C STEP 3 UT*Y=G
    DO 36 J=1,N
        S=0.0
        DO 34 I=1,M
            S=S+A(I,J)*Y(I)
34    CONTINUE
        G(J)=S
36    CONTINUE
C STEP 4
41    IF(Q.LT.0.0)STOP

```

```

C  STEP 5
      DO 56 J=1,N
        S=0.0
        DO 54 I=1,N
          IF(Z(I).GT.Q)S=S+V(J,I)*G(I)/Z(I)
54      CONTINUE
          X(J)=S
56      CONTINUE
C  STEP 6
C  NEW TOLERANCE VIA NEW CALL
      RETURN
      END

```

Example output

```

gfortran ../fortran/dr0102.f
mv ./a.out ../fortran/dr0102.run
../fortran/dr0102.run < ../fortran/dr0102.txt

```

```

##      0.10000000E+01  0.20000000E+01  0.30000000E+01  0.40000000E+01
## SING. VALS. .LE.  0.99999997E-05  ARE PRESUMED ZERO
##      3 ROTATIONS
##      3 ROTATIONS
##      1 ROTATIONS
##      0 ROTATIONS
## SV( 1)=  1.37529879E+01
## SV( 2)=  1.68960798E+00
## SV( 3)=  1.18504076E-05
## SINGULAR VALUE( 1)=  1.37529879E+01
## SINGULAR VALUE( 2)=  1.68960798E+00
## SINGULAR VALUE( 3)=  1.18504076E-05
## X( 1)=  1.00434840E+00
## X( 2)= -4.34857607E-03
## X( 3)= -4.02174187E+00

```

Special implementations

Most singular value decomposition codes are much, much more complicated than Algorithm 1 of the Nashlib collection. For some work on the magnetic field of Jupiter for NASA, Sidey Timmins has used an extended (quad) precision version of the method. One of us (JN) has converted an updated algorithm (Nash and Shlien (1987)) to the Fortran 95 dialect so the multiple precision FM Fortran tools of David M. Smith (see <http://dmsmith.lmu.build/>).

?? include this code and example in the repo??

BASIC

Listing

```

5 PRINT "dr0102.bas -- Nashlib Alg 01 and 02 driver"
10 PRINT "from ENHSVA APR 7 80 -- MOD 850519, remod 210113"
20 LET E1=1.0E-7
30 PRINT "ONE SIDED TRANSFORMATION METHOD FOR REGRESSIONS VIA"
40 PRINT "THE SINGULAR VALUE DECOMPOSITION -- J.C.NASH 1973,79"
150 LET M=4

```

```

160 LET N=3
210 DIM Y(M,N+1),A(M,N),T(N,N),G(N),X(N),Z(N),U(N),B(M)
220 DIM F$(10)
230 LET F$="K"
236 PRINT "Prep matrix and RHS"
240 LET Y(1,1)=5
241 LET Y(1,2)=1.0E-6
242 LET Y(1,3)=1
243 LET B(1)=1
250 LET Y(2,1)=6
251 LET Y(2,2)=0.999999
252 LET Y(2,3)=1
253 LET B(2)=2
260 LET Y(3,1)=7
261 LET Y(3,2)=2.00001
262 LET Y(3,3)=1
263 LET B(3)=3
270 LET Y(4,1)=8
271 LET Y(4,2)=2.9999
272 LET Y(4,3)=1
273 LET B(4)=4
500 FOR I=1 TO M
510 FOR J=1 TO N-1
520 LET A(I,J)=Y(I,J)
530 NEXT J
535 quit
540 LET A(I,N)=E3
550 NEXT I
560 LET E2=N*N*E1*E1
570 PRINT
580 FOR I=1 TO N
590 FOR J=1 TO N
600 LET T(I,J)=0
610 NEXT J
620 LET T(I,I)=1
630 NEXT I
640 LET I9=0
650 IF N=1 THEN GOTO 1150
660 LET N2=N*(N-1)/2
670 LET N1=N-1
680 LET N9=N2
690 LET I9=I9+1
700 FOR J=1 TO N1
710 LET J1=J+1
720 FOR K=J1 TO N
730 LET P=0
740 LET Q=0
750 LET R=0
760 FOR I=1 TO M
770 LET P=P+A(I,J)*A(I,K)
780 LET Q=Q+A(I,J)*A(I,J)
790 LET R=R+A(I,K)*A(I,K)
800 NEXT I

```



```

810 IF Q>=R THEN GOTO 850
820 LET C=0
830 LET S=1
840 GOTO 920
850 IF (Q*R)<=0 THEN GOTO 1040
860 IF P*P/(Q*R)<E2 THEN GOTO 1040
870 LET Q=Q-R
880 LET P=2*P
890 LET V1=SQR(P*P+Q*Q)
900 LET C=SQR((V1+Q)/(2*V1))
910 LET S=P/(2*V1*C)
920 FOR I=1 TO M
930 LET V1=A(I,J)
940 LET A(I,J)=V1*C+A(I,K)*S
950 LET A(I,K)=-V1*S+A(I,K)*C
960 NEXT I
970 FOR I=1 TO N
980 LET V1=T(I,J)
990 LET T(I,J)=V1*C+T(I,K)*S
1000 LET T(I,K)=-V1*S+T(I,K)*C
1010 NEXT I
1020 LET N9=N2
1030 GOTO 1060
1040 LET N9=N9-1
1050 IF N9=0 THEN GOTO 1150
1051 REM ?? GOTO was EXIT for NS BASIC
1060 NEXT K
1070 NEXT J
1080 PRINT "SWEEP",I9,
1090 IF O1>0 THEN PRINT #01,"SWEEP ",I9," ",
1100 IF 6*INT(I9/6)<>I9 THEN GOTO 680
1110 IF O1>0 THEN PRINT #01
1120 IF I9>=30 THEN GOTO 1150
1130 PRINT
1140 GOTO 680
1150 PRINT
1160 IF O1>0 THEN PRINT #01
1170 PRINT "CONVERGENCE AT SWEEP ",I9
1180 IF O1>0 THEN PRINT #01,"CONVERGENCE AT SWEEP ",I9
1190 FOR J=1 TO N
1200 LET Q=0
1210 FOR I=1 TO M
1220 LET Q=Q+A(I,J)^2
1230 NEXT I
1240 LET Q=SQR(Q)
1250 IF Q=0 THEN GOTO 1290
1260 FOR I=1 TO M
1270 LET A(I,J)=A(I,J)/Q
1280 NEXT I
1290 LET Z(J)=Q
1300 NEXT J
1310 PRINT
1320 PRINT "SINGULAR VALUES"

```

```

1340 FOR J=1 TO N
1350 PRINT Z(J),
1370 IF 5*INT(J/5)<>J THEN GOTO 1400
1380 PRINT
1400 NEXT J
1410 PRINT
1430 PRINT "VARIABLE # OF REGRESSAND",
1440 INPUT M2
1450 IF M2<=0 THEN GOTO 350
1470 LET S1=0
1480 FOR I=1 TO M
1490 LET S1=S1+(Y(I,M2)-E3*Y(M+1,M2))^2
1500 NEXT I
1510 FOR J=1 TO N
1520 LET S=0
1530 FOR I=1 TO M
1540 LET S=S+A(I,J)*Y(I,M2)
1550 NEXT I
1560 LET G(J)=S
1570 NEXT J
1580 PRINT "ENTER TOLERANCE FOR ZERO",
1590 INPUT Q
1600 IF Q<0 THEN GOTO 1410
1610 PRINT "SINGULAR VALUES <=",Q," ARE TAKEN AS 0"
1630 LET R=0
1640 FOR I=1 TO N
1650 LET V1=0
1660 LET S=0
1670 LET P=0
1680 FOR K=1 TO N
1690 LET C=0
1700 IF Z(K)<=Q THEN GOTO 1730
1710 LET C=1/Z(K)
1720 LET V1=V1+1
1730 LET S=S+C*T(I,K)*G(K)
1740 LET P=P+(C*T(I,K))^2
1750 NEXT K
1760 LET U(I)=P
1770 LET X(I)=S
1780 LET R=R+S*S
1790 NEXT I
1800 LET X(N)=X(N)*E3
1810 PRINT
1820 PRINT "RESIDUALS"
1840 LET C=0
1850 LET S2=0
1860 FOR I=1 TO M
1870 LET S=Y(I,M2)-X(N)
1880 FOR K=1 TO N-1
1890 LET S=S-Y(I,W(K))*X(K)
1900 NEXT K
1910 PRINT S,
1930 IF 5*INT(I/5)<>I THEN GOTO 1960

```

```

1940 PRINT
1960 LET C=C+S*S
1970 IF I=1 THEN GOTO 1990
1980 LET S2=S2+(S-S3)^2
1990 LET S3=S
2000 NEXT I
2010 PRINT
2020 LET P=0
2040 IF M<=V1 THEN GOTO 2060
2050 LET P=C/(M-V1)
2060 PRINT M-V1," DEGREES OF FREEDOM"
2080 REM PRINT
2090 PRINT "SOLUTION VECTOR - CONSTANT LAST"
2110 FOR I=1 TO N
2120 LET V1=SQR(P*U(I))
2130 PRINT "X(",W(I),")=",X(I)," STD.ERR.=" ,V1,
2140 IF O1>0 THEN PRINT #01,"X(",W(I),")=",X(I)," STD.ERR.=" ,V1,
2150 IF V1<=0 THEN GOTO 2180
2160 PRINT " T=",ABS(X(I)/V1),
2170 IF O1>0 THEN PRINT #01," T=",ABS(X(I)/V1),
2180 PRINT
2190 IF O1>0 THEN PRINT #01
2200 NEXT I
2210 PRINT "SUM OF SQUARES",C," SIGMA^2",P
2220 IF O1>0 THEN PRINT #01,"SUM OF SQUARES",C," SIGMA^2",P
2230 PRINT "NORM OF SOLUTION",SQR(R)
2240 IF O1>0 THEN PRINT #01,"NORM OF SOLUTION",SQR(R)
2250 PRINT "R SQUARED=",1-C/S1," DURBIN-WATSON STAT.=" ,S2/C
2260 IF O1>0 THEN PRINT #01,"R SQUARED=",1-C/S1," DURBIN-WATSON STAT.=" ,S2/C
2270 PRINT
2280 IF O1>0 THEN PRINT #01
2290 GOTO 1580
2300 REM GET SERIES FROM FILE
2310 PRINT "FILENAME OR 'KEYBOARD' OR 'K'",
2320 INPUT G$
2330 IF LEN(G$)>0 THEN LET F$=G$
2331 REM DEFAULTS TO LAST SETTING
2340 PRINT "DATA FROM FILE :",F$
2350 IF F$="KEYBOARD" THEN 2420
2360 IF F$<>"K" THEN 2460
2370 PRINT
2380 PRINT "ENTER SERIES"
2390 FOR I=1 TO M
2400 INPUT1 Y(I,J)
2410 IF 5*INT(I/5)=I THEN PRINT
2420 NEXT I
2430 PRINT
2440 IF O1>0 THEN GOSUB 2860
2450 RETURN
2460 IF FILE(F$)=3 THEN 2490
2470 PRINT "FILE NOT FOUND OR OF WRONG TYPE"
2480 GOTO 2310
2490 OPEN #1,F$

```

```

2500 PRINT "SERIES NAME OR #",
2510 INPUT X$
2520 IF X$(1,1)="#" THEN 2770
2530 IF TYP(1)=0 THEN 2740
2540 IF TYP(1)=1 THEN 2570
2550 READ #1,C
2560 GOTO 2530
2570 READ #1,Y$
2580 IF X$<>Y$ THEN 2530
2590 I=0
2600 PRINT "SERIES:",Y$
2610 IF O1>0 THEN PRINT #01,"SERIES:",Y$
2620 IF TYP(1)<>2 THEN 2690
2630 IF I=M THEN 2690
2640 I=I+1
2650 READ#1,Y(I,J)
2660 PRINT Y(I,J),
2670 IF 5*INT(I/5)=I THEN PRINT
2680 GOTO 2620
2690 PRINT
2700 PRINT "END OF SERIES  ",I," DATA POINTS"
2710 IF O1>0 THEN GOSUB 2860
2720 CLOSE #1
2730 RETURN
2740 PRINT "END OF FILE"
2750 CLOSE #1
2760 GOTO 2310
2770 X$=X$(2)
2780 P1=VAL(X$)
2790 J=0
2800 IF TYP(1)=0 THEN 2740
2810 IF TYP(1)=1 THEN 2840
2820 READ#1,C
2830 GOTO 2800
2840 J=J+1
2850 READ#1,Y$
2860 FOR I=1 TO M
2870 PRINT #01,Y(I,J),
2880 IF 5*INT(I/5)=I THEN PRINT #01
2890 NEXT I
2900 PRINT #01
2910 RETURN

```

Example output

```

bwbasic ../BASIC/dr0102.bas
echo "done"

```

```

## Bywater BASIC Interpreter/Shell, version 2.20 patch level 2
## Copyright (c) 1993, Ted A. Campbell
## Copyright (c) 1995-1997, Jon B. Volkoff
##
## dr0102.bas -- Nashlib Alg 01 and 02 driver
## from ENHSVA APR 7 80 -- MOD 850519, remod 210113

```

```

## ONE SIDED TRANSFORMATION METHOD FOR REGRESSIONS VIA
## THE SINGULAR VALUE DECOMPOSITION -- J.C.NASH 1973,79
## Prep matrix and RHS
##
## done

```

Pascal

Listing

```

Program runsvd(input,output);
{dr0102.pas == Calculation of Singular values and vectors of an arbitrary
  real matrix, solution of linear least squares approximation
  problem.

  Modifies a method due to Kaiser. See Nash and Shlien (1987): Simple
  algorithms for the partial singular value decomposition. Computer
  Journal, vol.30, pp.268-275.

  Modified for Turbo Pascal 5.0

  Copyright 1988, 1990 J.C.Nash
}

{constype.def ==
  This file contains various definitions and type statements which are
  used throughout the collection of "Compact Numerical Methods". In many
  cases not all definitions are needed, and users with very tight memory
  constraints may wish to remove some of the lines of this file when
  compiling certain programs.

  Modified for Turbo Pascal 5.0

  Copyright 1988, 1990 J.C.Nash
}
uses Dos, Crt; {Turbo Pascal 5.0 Modules}
{ 1. Interrupt, Unit, Interface, Implementation, Uses are reserved words now.}
{ 2. System,Dos,Crt are standard unit names in Turbo 5.0.}

const
  big = 1.0E+35;    {a very large number}
  Maxconst = 25;    {Maximum number of constants in data record}
  Maxobs = 100;     {Maximum number of observations in data record}
  Maxparm = 25;     {Maximum number of parameters to adjust}
  Maxvars = 10;     {Maximum number of variables in data record}
  acctol = 0.0001;  {acceptable point tolerance for minimisation codes}
  maxm = 20;        {Maximum number or rows in a matrix}
  maxn = 20;        {Maximum number of columns in a matrix}
  maxmn = 40;       {maxn+maxm, the number of rows in a working array}
  maxsym = 210;     {maximum number of elements of a symmetric matrix
                    which need to be stored = maxm * (maxm + 1)/2 }
  reltest = 10.0;   {a relative size used to check equality of numbers.
                    Numbers x and y are considered equal if the

```

```

        floating-point representation of reltest+x equals
        that of reltest+y.}
stepredn = 0.2;    {factor to reduce stepsize in line search}
yearwrit = 1990;  {year in which file was written}

type
str2 = string[2];
rmatrix = array[1..maxm, 1..maxn] of real; {a real matrix}
wmatrix = array[1..maxmn, 1..maxn] of real; {a working array, formed
        as one real matrix stacked on another}
smatvec = array[1..maxsym] of real; {a vector to store a symmetric matrix
        as the row-wise expansion of its lower triangle}
rvector = array[1..maxm] of real; {a real vector. We will use vectors
        of m elements always. While this is NOT space efficient,
        it simplifies program codes.}
cgmethodtype= (Fletcher_Reeves,Polak_Ribiere,Beale_Sorenson);
        {three possible forms of the conjugate gradients updating formulae}
probddata = record
    m      : integer; {number of observations}
    nvar   : integer; {number of variables}
    nconst : integer; {number of constants}
    vconst : array[1..Maxconst] of real;
    Ydata  : array[1..Maxobs, 1..Maxvars] of real;
    nlls   : boolean; {true if problem is nonlinear least squares}
end;

{
NOTE: Pascal does not let us define the work-space for the function
within the user-defined code. This is a weakness of Pascal for this
type of work.
}
var {global definitions}
    banner      : string[80]; {program name and description}

function calceps:real;
{calceps.pas ==
    This function returns the machine EPSILON or floating point tolerance,
    the smallest positive real number such that 1.0 + EPSILON > 1.0.
    EPSILON is needed to set various tolerances for different algorithms.
    While it could be entered as a constant, I prefer to calculate it, since
    users tend to move software between machines without paying attention to
    the computing environment. Note that more complete routines exist.
}
var
    e,e0: real;
    i: integer;
begin {calculate machine epsilon}
    e0 := 1; i:=0;
    repeat
        e0 := e0/2; e := 1+e0; i := i+1;
    until (e=1.0) or (i=50); {note safety check}
    e0 := e0*2;
{ Writeln('Machine EPSILON =',e0);}
    calceps:=e0;

```

```

end; {calceps}

function resid(nRow, nCol: integer; A : rmatrix;
              Y: rvector; Bvec : rvector; print : boolean):real;
{resids.pas
  == Computes residuals and , if print is TRUE, displays them 7
  per line for the linear least squares problem. The sum of
  squared residuals is returned.

  residual vector = A * Bvec - Y
}
var
i, j: integer;
t1, ss : real;

begin
  if print then
    begin
      writeln('Residuals');
    end;
    ss:=0.0;
    for i:=1 to nRow do
      begin
        t1:=-Y[i]; {note form of residual is residual = A * B - Y }
        for j:=1 to nCol do
          t1:=t1+A[i,j]*Bvec[j];
          ss:=ss+t1*t1;
          if print then
            begin
              write(t1:10,' ');
              if (i = 7 * (i div 7)) and (i<nRow) then writeln;
            end;
          end; {loop on i}
        if print then
          begin
            writeln;
            writeln('Sum of squared residuals =',ss);
          end;
        resid:=ss
      end; {resids.pas == residual calculation for linear least squares}

Procedure matcopy(nRow ,nCol: integer; A: rmatrix; var B:wmatrix);
{matcopy.pas
  -- copies matrix A, nRow by nCol, into matrix B }
var i,j: integer;
begin
  for i:=1 to nRow do
    for j:=1 to nCol do
      B[i,j]:=A[i,j];
    end;{matcopy.pas}

```

```

Procedure PrtSVDResults( nRow, nCol:integer;
                        U, V: rmatrix; Z: rvector);
{psvdres.pas
 == routine to display svd results and print them to confile
}
var
    i, j : integer;

begin
    writeln(' Singular values and vectors:');
    for j := 1 TO nCol do
        begin
            writeln('Singular value (' ,j,') =', Z[j]);
            writeln('Principal coordinate (U:');
            for i := 1 to nRow do
                begin
                    write(U[i,j]:10:7);
                    if (7 * (i div 7) = i) and (i<nRow) then writeln;
                end;
            writeln;
            writeln('Principal component (V:');
            for i:=1 to nCol do
                begin
                    write(V[i,j]:10:7);
                    if (7 * (i div 7) = i) and (i<nCol) then writeln;
                end;
            writeln;
        end;
    end; {psvdres == print svd results via procedure PrtSVDResults }

```

```

Procedure svdtst( A, U, V: rmatrix; Z: rvector;
                 nRow, UCol, VCol: integer);
{svdtst.pas
 == This routine tests the results of a singular value
    decomposition calculation. The matrix A is presumed to contain
    the matrix of which the purported decomposition is

```

$$U \quad Z \quad V\text{-transpose}$$

This routine tests column orthogonality of U and V, row orthogonality of V, and the reconstruction suggested by the decomposition. It does not carry out the tests of the Moore-Penrose inverse A^+ , which can be computed as

$$A^+ := V \quad Z \quad U\text{-transpose}.$$

FORTTRAN codes for the conditions

$$\begin{aligned}
 A^+ A A^+ &= ? = A^+ \\
 A A^+ A &= ? = A \\
 (A^+ A)\text{-transpose} &= ? = A^+ A \\
 (A A^+)\text{-transpose} &= ? = A A^+
 \end{aligned}$$


```

    are given in Nash, J.C. and Wang, R.L.C. (1986)
}

var
  i,j,k:integer;
  t1: real;
  imax, jmax: integer;
  valmax: real;

begin
  writeln('Column orthogonality of U');
  valmax:=0.0;
  imax:=0;
  jmax:=0;
  for i:=1 to UCol do
    begin
      for j:=i to UCol do
        begin
          t1:=0.0; {accumulate inner products}
          if i=j then t1:=-1;
          for k:=1 to nRow do t1:=t1+U[k,i]*U[k,j];
          if abs(t1)>abs(valmax) then
            begin
              imax:=i; jmax:=j; valmax:=t1;
            end;
          end;
        end;
      end;
    end;
  writeln('Largest inner product is ',imax,', ',jmax,', ',valmax);
  writeln('Row orthogonality of U (NOT guaranteed in svd)');
  valmax:=0.0;
  imax:=0;
  jmax:=0;
  for i:=1 to nRow do
    begin
      for j:=i to nRow do
        begin
          t1:=0.0; {accumulate inner products}
          if i=j then t1:=-1;
          for k:=1 to UCol do t1:=t1+U[i,k]*U[j,k];
          if abs(t1)>abs(valmax) then
            begin
              imax:=i; jmax:=j; valmax:=t1;
            end;
          end;
        end;
      end;
    end;
  writeln('Largest inner product is ',imax,', ',jmax,', ',valmax);
  writeln('Column orthogonality of V');
  valmax:=0.0;
  imax:=0;
  jmax:=0;
  for i:=1 to VCol do
    begin
      for j:=i to VCol do

```

```

begin
  t1:=0.0; {accumulate inner products}
  if i=j then t1:=-1.0;
  for k:=1 to VCol do t1:=t1+V[k,i]*V[k,j];
  if abs(t1)>abs(valmax) then
    begin
      imax:=i; jmax:=j; valmax:=t1;
    end;
  end;
end;
writeln('Largest inner product is ',imax,', ',jmax, '=',valmax);
writeln('Row orthogonality of V');
valmax:=0.0;
imax:=0;
jmax:=0;
for i:=1 to VCol do
begin
  for j:=i to VCol do
    begin
      t1:=0.0; {accumulate inner products}
      if i=j then t1:=-1;
      for k:=1 to VCol do t1:=t1+V[i,k]*V[j,k];
      if abs(t1)>abs(valmax) then
        begin
          imax:=i; jmax:=j; valmax:=t1;
        end;
      end;
    end;
  end;
writeln('Largest inner product is ',imax,', ',jmax, '=',valmax);
writeln('Reconstruction of initial matrix');
valmax:=0.0;
imax:=0;
jmax:=0;
for i:=1 to nRow do
begin
  for j:=1 to VCol do
    begin
      t1:=0;
      for k:=1 to VCol do
        t1:=t1+U[i,k]*Z[k]*V[j,k]; { U * S * V-transpose}
      {writeln('A[' ,i, ', ',j, ']=' ,A[i,j], ' Recon. =' ,t1, ' error=' ,A[i,j]-t1);}
      if abs(A[i,j]-t1)>abs(valmax) then
        begin
          imax:=i; jmax:=j; valmax:=A[i,j]-t1;
        end;
      end;
    end;
  end;
writeln('Largest error is ',imax,', ',jmax, '=',valmax);
end; {svdtst.pas}

{I matrixin.pas} {input or generate a matrix of reals}
{I vectorin.pas} {input or generate a vector of reals}

```

```

procedure NashSVD(nRow, nCol: integer;
                 var W: wmatrix;
                 var Z: rvector);

var
  i, j, k, EstColRank, RotCount, SweepCount, slimit : integer;
  eps, e2, tol, vt, p, x0, y0, q, r, c0, s0, d1, d2 : real;

procedure rotate;
var
  ii : integer;

begin
  for ii := 1 to nRow+nCol do
    begin
      D1 := W[ii,j]; D2 := W[ii,k];
      W[ii,j] := D1*c0+D2*s0; W[ii,k] := -D1*s0+D2*c0
    end;
  end;

begin
  writeln('alg01.pas -- NashSVD');
  eps := Calceps;
  slimit := nCol div 4; if slimit<6 then slimit := 6;

  SweepCount := 0;
  e2 := 10.0*nRow*eps*eps;
  tol := eps*0.1;

  EstColRank := nCol; ;

  for i := 1 to nCol do
    begin
      for j := 1 to nCol do
        W[nRow+i,j] := 0.0;
      W[nRow+i,i] := 1.0;
    end;

  repeat
    RotCount := EstColRank*(EstColRank-1) div 2;
    SweepCount := SweepCount+1;

    for j := 1 to EstColRank-1 do
      begin
        for k := j+1 to EstColRank do
          begin
            p := 0.0; q := 0.0; r := 0.0;
            for i := 1 to nRow do
              begin
                x0 := W[i,j]; y0 := W[i,k];
                p := p+x0*y0; q := q+x0*x0; r := r+y0*y0;
              end;
            end;

```

```

Z[j] := q; Z[k] := r;

if q >= r then
begin
  if (q<=e2*Z[1]) or (abs(p)<= tol*q) then RotCount := RotCount-1

  else
  begin
    p := p/q; r := 1-r/q; vt := sqrt(4*p*p + r*r);
    c0 := sqrt(0.5*(1+r/vt)); s0 := p/(vt*c0);
    rotate;
  end
end
else
begin

  p := p/r; q := q/r-1; vt := sqrt(4*p*p + q*q);
  s0 := sqrt(0.5*(1-q/vt));
  if p<0 then s0 := -s0;
  c0 := p/(vt*s0);
  rotate;
end;

end;
end;
writeln('End of Sweep #', SweepCount,
        '- no. of rotations performed =', RotCount);
while (EstColRank >= 3) and (Z[EstColRank] <= Z[1]*tol + tol*tol)
do EstColRank := EstColRank-1;
until (RotCount=0) or (SweepCount>slimit);
if (SweepCount > slimit) then writeln('**** SWEEP LIMIT EXCEEDED');
end;

procedure svdlss(nRow, nCol: integer;
                 W : wmatrix;
                 Y: rvector;
                 Z : rvector;
                 A : rmatrix;
                 var Bvec: rvector;
                 q : real);

var
  i, j, k : integer;
  s : real;

begin
  writeln('alg02.pas == svdlss');
{  write('Y:');
  for i := 1 to nRow do
  begin
    write(Y[i], ' ');
  end;
}

```

```

writeln;

for i := 1 to (nRow+nCol) do
begin
    write('W row ',i,':');
    for j:= 1 to nCol do
    begin
        write(W[i,j], ' ');
    end;
    writeln;
end;
}
{
    writeln('Singular values');
    for j := 1 to nCol do
    begin
        write(Z[j]:18, ' ');
        if j=4 * (j div 4) then writeln;
    end;
    writeln;
}

if q>=0.0 then
begin
    q := q*q;
    for i := 1 to nCol do
    begin
        s := 0.0;
        for j := 1 to nCol do
        begin
            for k := 1 to nRow do
            begin
                if Z[j]>q then
                    s := s + W[i+nRow,j]*W[k,j]*Y[k]/Z[j];
                    { V   S+   U'   y }

            end;
        end;
        Bvec[i] := s;
    end;
    writeln('Least squares solution');
    for j := 1 to nCol do
    begin
        write(Bvec[j]:12, ' ');
        if j=5 * (j div 5) then writeln;
    end;
    writeln;
    s := resids(nRow, nCol, A, Y, Bvec, true);
end;
end;

{main program}
var
    nRow, nCol : integer;
    A, V, U : rmatrix;

```

```

W : wmatrix; {a working matrix which will contain U Zd in the
upper nRow rows, and V in the bottom nCol rows, where Zd
is the diagonal matrix of singular values. That is, W
becomes

      ( U  Zd )
      (      )
      (      V  )

}
Z, Zsq : rvector; {Z will contain either the squares of singular
values or the singular values themselves}
Y : rvector; {Y will contain the 'right hand side' of the
least squares problem, i.e. the vector to be
approximated }
Bvec : rvector; {the least squares solution }
inchar : char;
i,j,k, imax, jmax : integer;
t1, t2: real;

begin
  banner:='dr0102.pas -- driver for svd and least squares solution';
  {Test matrix from CNM pg 34}
  nRow:=4;
  nCol:=3;
  {Read in matrix the hard way!}
  A[1,1]:=5; A[1,2]:=1.0E-6; A[1,3]:=1; Y[1]:=1;
  A[2,1]:=6; A[2,2]:=0.999999; A[2,3]:=1; Y[2]:=2;
  A[3,1]:=7; A[3,2]:=2.00001; A[3,3]:=1; Y[3]:=3;
  A[4,1]:=8; A[4,2]:=2.9999; A[4,3]:=1; Y[4]:=4;

  Matcopy(nRow,nCol, A, W); {The matrix A is copied into working array W.}
  NashSVD( nRow, nCol, W, Z); {The singular value decomposition is
    computed for matrix A by columnwise orthogonalization of the
    working array W, to which a unit matrix of order nCol is added
    in order to form the matrix V in the bottom nCol rows of W.}
  begin
    for j:=1 to nCol do
      begin
        Zsq[j] := Z[j];
        Z[j]:= sqrt(Z[j]);
        for i:=1 to nRow do U[i,j]:=W[i,j]/Z[j];
        for i:=1 to nCol do V[i,j]:=W[i+nRow,j];
      end;
    PrtSVDResults( nRow, nCol, U, V,Z);
    begin
      svdtst(A,U,V,Z,nRow,nCol,nCol);
      writeln('Reconstruction of initial matrix from Nash working form');
      t2:=0.0; {to store largest error in reconstruction}
      for i:=1 to nRow do
        begin
          for j:=1 to nCol do
            begin

```

```

    t1:=0.0;
    for k:=1 to nCol do
        t1:=t1+W[i,k]*W[j+nRow,k]; { U * S * V-transpose}
    t1:=A[i,j]-t1; {to compute the residual}
    if abs(t1)>t2 then
    begin
        t2:=abs(t1); imax:=i; jmax:=j; {to save biggest element}
    end;
    end; {loop over columns}
end; {loop over rows}
writeln('Largest error is ',imax,',',jmax,'=',t2);
end; {test svd results}
end; {print results}
svdlss(nRow, nCol, W, Y, Zsq, A, Bvec, 1.0e-16);
end. {dr0102.pas == svd and least squares solution}

```

Example output

For some reason not yet understood, running the compiled Pascal program does not transfer the output to our Rmarkdown output, so we resort to saving the output and then listing it as we do program code.

```

fpc ../Pascal2021/dr0102.pas
mv ../Pascal2021/dr0102 ../Pascal2021/dr0102.run
# now execute it
../Pascal2021/dr0102.run > ../Pascal2021/dr0102.out

```

```

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr0102.pas
## dr0102.pas(487,3) Note: Local variable "inchar" not used
## Linking ../Pascal2021/dr0102
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 538 lines compiled, 0.1 sec
## 1 note(s) issued

```

```

alg01.pas -- NashSVD
End of Sweep #1- no. of rotations performed =3
End of Sweep #2- no. of rotations performed =3
End of Sweep #3- no. of rotations performed =1
End of Sweep #4- no. of rotations performed =0
Singular values and vectors:
Singular value (1) = 1.3752987437308155E+001
Principal coordinate (U):
0.3589430 0.4465265 0.5341101 0.6216916
Principal component (V):
0.9587864 0.2457477 0.1426069
Singular value (2) = 1.6896078122466185E+000
Principal coordinate (U):
-0.7557625-0.3171936 0.1213826 0.5598907
Principal component (V):
-0.2090249 0.9500361-0.2318187
Singular value (3) = 1.1885323302979959E-005
Principal coordinate (U):
-0.3286873 0.1117406 0.7626745-0.5457163

```

```

Principal component (V):
-0.1924506 0.1924563 0.9622491
Column orthogonality of U
Largest inner product is 1,3= 2.8635982474156663E-011
Row orthogonality of U (NOT guaranteed in svd)
Largest inner product is 2,2=-6.8751638785273139E-001

Column orthogonality of V

Largest inner product is 3,3=-1.1102230246251565E-016

Row orthogonality of V

Largest inner product is 3,3=-1.1102230246251565E-016

Reconstruction of initial matrix

Largest error is 4,1=-1.7763568394002505E-015

Reconstruction of initial matrix from Nash working form

Largest error is 4,1= 1.7763568394002505E-015

alg02.pas == svdlss

Least squares solution

1.0000E+000 2.4766E-006 -4.0000E+000

Residuals

-9.21E-011 -2.43E-011 7.57E-011 -1.24E-010

Sum of squared residuals = 3.0174571907166908E-020

```

For some reason, we get extra line-feed characters in the output file. They are easily removed with a text editor from the output file, but their origin is unclear. JN 2021-1-20 ??

Python

Pending ...

R

Listing

While based on Nash and Shlien (1987), the following code shows that R can be used quite easily to implement Algorithm 1. The least squares solution (Algorithm 2) is embedded in the example output.

```

Nashsvd <- function(A, MaxRank=0, cyclelimit=25, trace = 0, rotnchk=0.3) {
  ## Nashsvd.R -- An attempt to remove tolerances from Nash & Shlien algorithm 190327
  # Partial svd by the one-sided Jacobi method of Nash & Shlien
  # Computer Journal 1987 30(3), 268-275
  # Computer Journal 1975 18(1) 74-76
  if (cyclelimit < 6) {

```



```

warning("Nashsvd: You cannot set cyclelimit < 6 without modifying the code")
cyclelimit <- 6 # safety in case user tries smaller
}
m <- dim(A)[1]
n <- dim(A)[2]
if (MaxRank <= 0) MaxRank <- n
EstColRank <- n # estimated column rank
# Note that we may simply run algorithm to completion, or fix the
# number of columns by EstColRank. Need ?? to fix EstColRank=0 case.??
V <- diag(nrow=n) # identity matrix in V
if (is.null(EstColRank)) {EstColRank <- n } # Safety check on number of sv's
z <- rep(NA, n) # column norm squares -- safety setting
keepgoing <- TRUE
SweepCount <- 0
while (keepgoing) { # main loop of repeating cycles of Jacobi
  RotCount <- 0
  SweepCount <- SweepCount + 1
  if (trace > 1) cat("Sweep:", SweepCount, "\n")
  ## if (EstColRank == n) { EstColRank <- n - 1 } # safety
  for (jj in 1:(EstColRank-1)) { # left column indicator
    for (kk in (jj+1): n) { # right hand column
      p <- q <- r <- 0.0 #
      oldjj <- A[,jj]
      oldkk <- A[,kk]
      p <- as.numeric(crossprod(A[,jj], A[,kk]))
      q <- as.numeric(crossprod(A[,jj], A[,jj]))
      r <- as.numeric(crossprod(A[,kk], A[,kk]))
      if (trace > 2) cat(jj, " ", kk, ": pqr", p, " ", q, " ", r, " ")
      z[jj] <- q
      z[kk] <- r
      if (q >= r) { # in order, so can do test of "convergence" -- change to 0.2 * abs(p) for odd ca
        if ( (as.double(z[1]+q) > as.double(z[1])) && (as.double(rotnchk*abs(p)+q) > as.double(q))
          RotCount <- RotCount + 1
          p <- p/q
          r <- 1 - (r/q)
          vt <- sqrt(4*p*p + r*r)
          c0 <- sqrt(0.5*(1+r/vt))
          s0 <- p/(vt*c0)
          # rotate
          cj <- A[,jj]
          ck <- A[,kk]
          A[,jj] <- c0*cj + s0*ck
          A[,kk] <- -s0*cj + c0*ck
          cj <- V[,jj]
          ck <- V[,kk]
          V[,jj] <- c0*cj + s0*ck
          V[,kk] <- -s0*cj + c0*ck
        } else {
          if (trace > 2) cat(" NO rotn ")
        }
      } else { # out of order, must rotate
        if (trace > 2) cat("|order|")
        RotCount <- RotCount + 1

```

```

    p <- p/r
    q <- (q/r) - 1.0
    vt <- sqrt(4*p*p + q*q)
    s0 <- sqrt(0.5*(1-q/vt))
    if (p < 0) { s0 <- -s0 }
    c0 <- p/(vt*s0)
    # rotate
    cj <- A[,jj]
    ck <- A[,kk]
    A[,jj] <- c0*cj + s0*ck
    A[,kk] <- -s0*cj + c0*ck
    cj <- V[,jj]
    ck <- V[,kk]
    V[,jj] <- c0*cj + s0*ck
    V[,kk] <- -s0*cj + c0*ck
  } # end q >= r test
  nup <- as.numeric(crossprod(A[,jj], A[,kk]))
#   nuq <- as.numeric(crossprod(A[,jj], A[,jj]))
#   nur <- as.numeric(crossprod(A[,kk], A[,kk]))
  if (trace > 2) cat("    new: p= ", nup, " Rel: ", nup*nup/z[1], "\n")
} # end kk
} # end jj
if (trace > 0) {cat("End sweep ", SweepCount, "  No. rotations =", RotCount, "\n")}
if (trace > 2) tmp <- readline("cont.?\n")
while ( (EstColRank >= 3) && (as.double(sqrt(z[EstColRank]))+sqrt(z[1]) == as.double(sqrt(z[1])) ))
# ?? Why can we not use 2? Or do we need at least 2 cols
  EstColRank <- EstColRank - 1
  if (trace > 0) {cat("Reducing rank to ", EstColRank, "\n")} # ?? can do this more cleanly
} # end while for rank estimation
## Here may want to adjust for MaxRank. How??
if (MaxRank < EstColRank) {
  if (trace > 0) {
    cat("current estimate of sv[", MaxRank, "/sv[1] =", sqrt(z[MaxRank]/z[1]), "\n")
    cat("reducing rank by 1\n")
  }
  EstColRank <- EstColRank - 1
}
if (SweepCount >= cyclelimit) {
  if (trace > 0) cat("Cycle limit reached\n")
  keepgoing <- FALSE
}
if (RotCount == 0) {
  if (trace > 1) cat("Zero rotations in cycle\n")
  keepgoing <- FALSE
}
} # End main cycle loop
z <- sqrt(z)
A <- A %*% diag(1/z)
ans <- list( d = z, u = A, v = V, cycles=SweepCount, rotations=RotCount)
ans
} # end partsvd()

```

Example output

```
# test taken from dr0102.pas
```

```
A<-matrix(0, 4,3)
A[1,]<-c(5, 1e-6, 1)
A[2,]<-c(6, 0.999999, 1)
A[3,]<-c(7, 2.00001, 1)
A[4,]<-c(8, 2.9999, 1)
print(A)
```

```
##      [,1]      [,2] [,3]
## [1,]    5 0.000001    1
## [2,]    6 0.999999    1
## [3,]    7 2.000010    1
## [4,]    8 2.999900    1
```

```
b<-c(1,2,3,4)
print(b)
```

```
## [1] 1 2 3 4
```

```
# try the R-base svd
```

```
sA <- svd(A)
sA
```

```
## $d
## [1] 1.375299e+01 1.689608e+00 1.188532e-05
##
## $u
##      [,1]      [,2]      [,3]
## [1,] -0.3589430 -0.7557625  0.3286873
## [2,] -0.4465265 -0.3171936 -0.1117406
## [3,] -0.5341101  0.1213826 -0.7626745
## [4,] -0.6216916  0.5598907  0.5457163
##
## $v
##      [,1]      [,2]      [,3]
## [1,] -0.9587864 -0.2090249  0.1924506
## [2,] -0.2457477  0.9500361 -0.1924563
## [3,] -0.1426069 -0.2318187 -0.9622491
```

```
yy <- t(sA$u) %*% as.matrix(b)
xx <- sA$v %*% diag(1/sA$d) %*% yy
xx
```

```
##      [,1]
## [1,] 1.000000e+00
## [2,] -9.005019e-12
## [3,] -4.000000e+00
```

```
# Now the Nashsvd code (this is likely NOT true to 1979 code)
```

```
source("../R/Nashsvd.R")
nsvd <- Nashsvd(A)
print(nsvd)
```

```
## $d
## [1] 1.375299e+01 1.689608e+00 1.188532e-05
##
```

```

## $u
##           [,1]      [,2]      [,3]
## [1,] 0.3589430 -0.7557625 -0.3286873
## [2,] 0.4465265 -0.3171936  0.1117406
## [3,] 0.5341101  0.1213826  0.7626745
## [4,] 0.6216916  0.5598907 -0.5457163
##
## $v
##           [,1]      [,2]      [,3]
## [1,] 0.9587864 -0.2090249 -0.1924506
## [2,] 0.2457477  0.9500361  0.1924563
## [3,] 0.1426069 -0.2318187  0.9622491
##
## $cycles
## [1] 4
##
## $rotations
## [1] 0

# Note least squares solution can be done by matrix multiplication
U <- nsvd$u
V <- nsvd$v
d <- nsvd$d
di <- 1/d
di <- diag(di) # convert to full matrix -- note entry sizes
print(di)

##           [,1]      [,2]      [,3]
## [1,] 0.07271147 0.0000000  0.00
## [2,] 0.00000000 0.5918533  0.00
## [3,] 0.00000000 0.0000000 84137.38

lsol <- t(U) %*% b
lsol <- di %*% lsol
lsol <- V %*% lsol
print(lsol)

##           [,1]
## [1,] 9.999975e-01
## [2,] 2.476918e-06
## [3,] -3.999988e+00

res <- b - A %*% lsol
print(res)

##           [,1]
## [1,] 5.027934e-11
## [2,] -1.708989e-11
## [3,] -1.166609e-10
## [4,] 8.347678e-11

cat("sumsquares = ", as.numeric(crossprod(res)))

## sumsquares = 2.339822e-20

# now set smallest singular value to 0 and in pseudo-inverse
dix <- di

```

```
dix[3,3] <- 0
lsolx <- V %*% dix %*% t(U) %*% b
# this gives a very different least squares solution
print(lsolx)
```

```
##           [,1]
## [1,]  0.2222209
## [2,]  0.7778018
## [3,] -0.1111212
```

```
# but the residuals (in this case) are nearly 0 too
resx <- b - A %*% lsolx
cat("sumsquares = ", as.numeric(crossprod(resx)))
```

```
## sumsquares =  2.307256e-09
```

Others

Pending ...

?? Could we f2c the Fortran and manually tweak to get a C code?

There is also a C version in

<https://github.com/LuaDist/gsl/blob/master/linalg/svd.c>

=====

Algorithm 3 – Givens’ decomposition

The Givens and Householder decompositions of a rectangular m by n matrix A ($m \geq n$) both give an m by m orthogonal matrix Q and an upper-triangular n by n matrix R whose product QR is a close approximation of A . At the time Nash (1979) was being prepared, the Givens approach seemed to give a more compact program code, though neither approach is large.

In practice, if one is trying to solve linear equations

$$Ax = b$$

or linear least squares problems of the form

$$Ax = b$$

then the right hand side (RHS) b can be appended to the matrix A so that the resulting working matrix

$$W = [A|b]$$

is transformed during the formation of the Q matrix into

$$W_{trans} = [R|Q'b]$$

This saves us the effort of multiplying b by the transpose of Q before we back-solve for x .

In fact, m does not have to be greater than or equal to n . However, underdetermined systems of equations do raise some issues that we will not address here.

It is therefore unnecessary to store Q , which when Nash (1979) was being prepared was a potentially large matrix. There are alternative designs of the code which could save information on the plane rotations that make up Q . Such codes can then apply the rotations to a unit matrix of the right size to reconstruct Q as needed. However, these details have largely become irrelevant in an age of cheap memory chips.

Fortran

Listing

The following listing uses the Frank matrix as a test.

```
C&&& A3
C  TEST ALGORITHM 3
C  J.C. NASH    JULY 1978, APRIL 1989
      LOGICAL SAVEQ
      CHARACTER QSAVE
      INTEGER M,N,NIN,NOUT
      REAL A(10,10),Q(10,10),EPS,S,W(10,10)
      NDIM=10
C  I/O CHANNELS
      NIN=5
      NOUT=6
      1  READ(NIN,900)M,N,QSAVE
      900  FORMAT(2I5,A1)
      WRITE(NOUT,950)M,N,QSAVE
      950  FORMAT('M=',I5,' N=',I5,' QSAVE=',A1)
      IF(M.EQ.0.OR.N.EQ.0)STOP
      SAVEQ=.FALSE.
```

```

        IF (QSAVE .EQ. "T") SAVEQ=.TRUE.
        CALL FRANKM(M,N,A,10)
        WRITE(NOUT,952)
952  FORMAT('INITIAL MATRIX')
        CALL OUT(A,NDIM,M,N,NOUT)
        DO 10 I=1,M
            DO 5 J=1,N
C          COPY MATRIX TO WORKING ARRAY
            W(I,J)=A(I,J)
        5      CONTINUE
    10      CONTINUE
C  IBM MACHINE PRECISION
        EPS=16.0**(-5)
        CALL A3GR(M,N,W,10,Q,EPS,SAVEQ)
        WRITE(NOUT,953)
953  FORMAT('FULL DECOMPOSED MATRIX')
        CALL OUT(A,NDIM,M,N,NOUT)
        IF(SAVEQ)CALL A3DT(M,N,W,NDIM,Q,NOUT,A)
        GOTO 1
        END
        SUBROUTINE A3DT(M,N,W,NDIM,Q,NOUT,A)
C  TESTS GIVENS' DECOMPOSITION
C  J.C. NASH    JULY 1978, APRIL 1989
        INTEGER M,N,NDIM,NOUT,I,J,K
        REAL A(NDIM,N),Q(NDIM,M),W(NDIM,N),S,T
        WRITE(NOUT,960)
960  FORMAT(' Q MATRIX')
        CALL OUT(Q,NDIM,M,M,NOUT)
        WRITE(NOUT,961)
961  FORMAT(' R MATRIX (STORED IN W')
        CALL OUT(W,NDIM,M,N,NOUT)
        IF(N.LT.M)GOTO 9
        S=1.0
        DO 5 I=1,M
            S=S*W(I,I)
        5      CONTINUE
        WRITE(NOUT,963)S
963  FORMAT(' DETERMINANT=',1PE16.8)
        9      CONTINUE
        T=0.0
        DO 20 I=1,M
            DO 15 J=1,N
                S=0.0
                DO 10 K=1,M
                    S=S+Q(I,K)*W(K,J)
                10      CONTINUE
                S=S-A(I,J)
                IF(ABS(S).GT.T)T=ABS(S)
            15      CONTINUE
        20      CONTINUE
        WRITE(NOUT,962)T
962  FORMAT(' MAX. DEVN. OF RECONSTRUCTION FROM ORIGINAL=',E16.8)
        RETURN

```

```

        END
        SUBROUTINE OUT(A,NDIM,N,NP,NOUT)
C   J.C. NASH   JULY 1978, APRIL 1989
        INTEGER NDIM,N,NOUT,I,J
        REAL A(NDIM,NP)
        DO 20 I=1,N
            WRITE(NOUT,951)I
951    FORMAT(' ROW',I3)
            WRITE(NOUT,952)(A(I,J),J=1,NP)
952    FORMAT(1H ,1P5E16.8)
        20 CONTINUE
        RETURN
        END
        SUBROUTINE A3GR(M,N,A,NDIM,Q,EPS,SAVEQ)
C   ALGORITHM 3  GIVENS' REDUCTION
C   J.C. NASH   JULY 1978, FEBRUARY 1980, APRIL 1989
C   M,N   = ORDER OF MATRIX TO BE DECOMPOSED
C   A     = ARRAY CONTAINING MATRIX TO BE DECOMPOSED
C   NDIM  = FIRST DIMENSION OF MATRICES - NDIM.GE.M
C   Q     = ARRAY CONTAINING ORTHOGONAL MATRIX OF ACCUMULATED ROTATIONS
C   EPS   = MACHINE PRECISION = SMALLEST NO.GT.0.0 S.T. 1.0+EPS.GT.1.0
C   SAVEQ= LOGICAL FLAG SET .TRUE. IF Q TO BE FORMED
C   STEP 0
        LOGICAL SAVEQ
        INTEGER N,M,NA,MN,I,J,K,J1
        REAL A(NDIM,N),Q(NDIM,M),EPS,TOL,B,P,S,C
        MN=M
        IF(M.GT.N)MN=N
        IF(.NOT.SAVEQ)GOTO 9
        DO 5 I=1,M
            DO 4 J=1,M
                Q(I,J)=0.0
            4 CONTINUE
                Q(I,I)=1.0
        5 CONTINUE
        9 TOL=EPS*EPS
C   STEP 1
        IF(M.EQ.1)RETURN
        DO 100 J=1,MN
            J1=J+1
            IF(J1.GT.M)GOTO 100
C   STEP 2
            DO 90 K=J1,M
C   STEP 3
                C=A(J,J)
                S=A(K,J)
                B=ABS(C)
                IF(ABS(S).GT.B)B=ABS(S)
                IF(B.EQ.0.0)GOTO 90
                C=C/B
                S=S/B
                P=SQRT(C*C+S*S)
C   STEP 4

```



```

        S=S/P
C  STEP 5      IF(ABS(S).LT.TOL)GOTO 90
C  STEP 6      C=C/P
C  STEP 7
        DO 75 I=1,N
            P=A(J,I)
            A(J,I)=C*P+S*A(K,I)
            A(K,I)=-S*P+C*A(K,I)
75      CONTINUE
C  STEP 8      IF(.NOT.SAVEQ)GOTO 90
        DO 85 I=1,M
            P=Q(I,J)
            Q(I,J)=C*P+S*Q(I,K)
            Q(I,K)=-S*P+C*Q(I,K)
85      CONTINUE
C  STEP 9
90      CONTINUE
C  STEP 10
100     CONTINUE
        RETURN
        END
        SUBROUTINE FRANKM(M,N,A,NA)
C  J.C. NASH    JULY 1978, APRIL 1989
        INTEGER M,N,NA,I,J
C  INPUTS FRANK MATRIX M BY N INTO A
        REAL A(NA,N)
        DO 20 I=1,M
            DO 10 J=1,N
                A(I,J)=AMINO(I,J)
10      CONTINUE
20      CONTINUE
        RETURN
        END

```

Example output

As a precaution, we use a 1 by 1 matrix as our first test. We have seen situations where otherwise reliable programs have failed on such trivial cases.

```

gfortran ../fortran/a3.f
mv ./a.out ../fortran/a3.run
../fortran/a3.run < ../fortran/a3data.txt > ../fortran/a3out.txt

```

```

M=      1  N=      1  QSAVE=T
INITIAL MATRIX
ROW      1
      1.00000000E+00
FULL DECOMPOSED MATRIX
ROW      1
      1.00000000E+00
Q MATRIX
ROW      1

```

```

1.00000000E+00
R MATRIX (STORED IN W
ROW 1
1.00000000E+00
DETERMINANT= 1.00000000E+00
MAX. DEVN. OF RECONSTRUCTION FROM ORIGINAL= 0.00000000E+00
M= 5 N= 3 QSAVE=T
INITIAL MATRIX
ROW 1
1.00000000E+00 1.00000000E+00 1.00000000E+00
ROW 2
1.00000000E+00 2.00000000E+00 2.00000000E+00
ROW 3
1.00000000E+00 2.00000000E+00 3.00000000E+00
ROW 4
1.00000000E+00 2.00000000E+00 3.00000000E+00
ROW 5
1.00000000E+00 2.00000000E+00 3.00000000E+00
FULL DECOMPOSED MATRIX
ROW 1
1.00000000E+00 1.00000000E+00 1.00000000E+00
ROW 2
1.00000000E+00 2.00000000E+00 2.00000000E+00
ROW 3
1.00000000E+00 2.00000000E+00 3.00000000E+00
ROW 4
1.00000000E+00 2.00000000E+00 3.00000000E+00
ROW 5
1.00000000E+00 2.00000000E+00 3.00000000E+00
Q MATRIX
ROW 1
4.47213590E-01 -8.94427240E-01 9.95453036E-08 1.14146687E-07 -1.93894891E-08
ROW 2
4.47213590E-01 2.23606765E-01 -8.66025507E-01 0.00000000E+00 -1.19209290E-07
ROW 3
4.47213590E-01 2.23606795E-01 2.88675159E-01 -7.07106888E-01 -4.08248186E-01
ROW 4
4.47213590E-01 2.23606944E-01 2.88675249E-01 7.07106769E-01 -4.08248246E-01
ROW 5
4.47213590E-01 2.23606795E-01 2.88674951E-01 0.00000000E+00 8.16496611E-01
R MATRIX (STORED IN W
ROW 1
2.23606801E+00 4.02492237E+00 5.36656284E+00
ROW 2
1.92373264E-08 8.94427299E-01 1.56524777E+00
ROW 3
2.48352734E-08 1.40489522E-08 8.66025269E-01
ROW 4
4.86669869E-08 2.58095696E-08 0.00000000E+00
ROW 5
-1.40489469E-08 -4.96705121E-09 0.00000000E+00
MAX. DEVN. OF RECONSTRUCTION FROM ORIGINAL= 0.29802322E-06
M= 0 N= 0 QSAVE=

```

BASIC

Listing

The following listing also uses the Frank matrix as a test. The code has been adjusted for fixed input to allow it to be run within the `knitr` processor for Rmarkdown.

```
2 REM DIM A(10,10),Q(10,10)
10 PRINT "TEST GIVENS - GIFT - ALG 3"
12 LET M8=10
14 LET N8=10
20 DIM A(M8,N8),Q(M8,M8)
25 REM PRINT "M=",
30 REM INPUT M
32 LET M=5
40 REM PRINT "  N=",
50 REM INPUT N
52 LET N=3
70 GOSUB 1500
80 PRINT "ORIGINAL",
85 GOSUB 790
90 GOSUB 500 : REM GIVENS DECOMPOSITION
94 PRINT "FINAL ";
96 GOSUB 790
97 PRINT "FINAL ";
98 GOSUB 840
100 PRINT "RECOMBINATION "
110 FOR I=1 TO M
111   PRINT "ROW";I;":";
120   FOR J=1 TO N
130     LET S=0
140     FOR K=1 TO M
150       LET S=S+Q(I,K)*A(K,J)
160     NEXT K
170     PRINT S;" ";
210   NEXT J
220   PRINT
230 NEXT I
240 QUIT
245 REM STOP
500 REM GIVENS TRIANGULARIZATION
520 PRINT "GIVENS TRIANGULARIZATION DEC 12 77"
540 FOR I=1 TO M
545   FOR J=1 TO M
550     LET Q(I,J)=0
555   NEXT J
560   LET Q(I,I)=1
565 NEXT I
575 REM GOSUB 840: REM PRINT ORIGINAL Q MATRIX
580 LET E1=1E-7 : REM NORTH STAR 8 DIGIT -- can be changed!
585 LET T9=E1*E1
600 FOR J=1 TO N-1
605   FOR K=J+1 TO M
610     LET C=A(J,J)
615     LET S=A(K,J)
```

```

625     REM PRINT "J=",J," K=",K," A[J,J]=",C," A[K,J]=",S
630     REM PRINT "BYPASS SAFETY DIVISION ",
635     REM GOTO 660
640     LET B=ABS(C)
645     IF ABS(S)<=B THEN GOTO 655
650     LET B=ABS(S)
655     LET C=C/B
660     LET S=S/B
665     IF B=0 THEN GOTO 770
670     LET P=SQR(C*C+S*S)
680     LET S=S/P
685     IF ABS(S)<T9 THEN GOTO 770
690     LET C=C/P
695     FOR I=1 TO N
700         LET P=A(J,I)
705         LET A(J,I)=C*P+S*A(K,I)
710         LET A(K,I)=-S*P+C*A(K,I)
715     NEXT I
720     IF J=N-1 THEN GOTO 730
730     REM IF I5=0 THEN GOTO 770
735     FOR I=1 TO M
740         LET P=Q(I,J)
745         LET Q(I,J)=C*P+S*Q(I,K)
750         LET Q(I,K)=-S*P+C*Q(I,K)
755     NEXT I
770     REM Possible print point
775     NEXT K
780 NEXT J
785 RETURN
790 PRINT " A MATRIX"
795 FOR H=1 TO M
800     PRINT "ROW";H;": ";
805     FOR L=1 TO N
810         PRINT A(H,L);" ";
815     NEXT L
820     PRINT
825 NEXT H
830 PRINT
835 RETURN
840 PRINT " Q MATRIX"
845 FOR H=1 TO M
850     PRINT "ROW";H;": ";
855     FOR L=1 TO M
860         PRINT Q(H,L);" ";
865     NEXT L
870     PRINT
875 NEXT H
880 PRINT
885 RETURN
1500 REM PREPARE FRANK MATRIX IN A
1510 FOR I=1 TO M
1530 FOR J=1 TO N
1540 IF (I <= J) THEN LET A(I,J)=I ELSE LET A(I,J)=J

```

```

1550 NEXT J
1560 NEXT I
1570 RETURN
1600 END

```

Example output

As a precaution, we use a 1 by 1 matrix as our first test. We have seen situations where otherwise reliable programs have failed on such trivial cases.

```
bwbasic ../BASIC/a3.bas
```

```

## Bywater BASIC Interpreter/Shell, version 2.20 patch level 2
## Copyright (c) 1993, Ted A. Campbell
## Copyright (c) 1995-1997, Jon B. Volkoff
##
## TEST GIVENS - GIFT - ALG 3
## ORIGINAL
##   A MATRIX
## ROW 1: 1  1  1
## ROW 2: 1  2  2
## ROW 3: 1  2  3
## ROW 4: 1  2  3
## ROW 5: 1  2  3
##
## GIVENS TRIANGULARIZATION DEC 12 77
## FINAL   A MATRIX
## ROW 1: 2.2360680  4.0249224  5.3665631
## ROW 2: 0  0.8944272  1.5652476
## ROW 3: 0  0  0.7071068
## ROW 4: 0  0  0.4082483
## ROW 5: -0  -0  0.2886751
##
## FINAL   Q MATRIX
## ROW 1: 0.4472136  -0.8944272  0  0  0
## ROW 2: 0.4472136  0.2236068  -0.7071068  -0.4082483  -0.2886751
## ROW 3: 0.4472136  0.2236068  0.7071068  -0.4082483  -0.2886751
## ROW 4: 0.4472136  0.2236068  0  0.8164966  -0.2886751
## ROW 5: 0.4472136  0.2236068  0  0  0.8660254
##
## RECOMBINATION
## ROW 1: 1  1  1
## ROW 2: 1  2  2.0000000
## ROW 3: 1  2  3
## ROW 4: 1.0000000  2.0000000  3.0000000
## ROW 5: 1.0000000  2.0000000  3.0000000

```

Pascal

Listing – column-wise approach

```

program givrun(input, output);
{dr03.PAS == driver for Givens' reduction of a matrix

    Copyright 1988 J.C.Nash

```

```

}
{I constype.def}
{constype.def ==
    This file contains various definitions and type statements which are
    used throughout the collection of "Compact Numerical Methods". In many
    cases not all definitions are needed, and users with very tight memory
    constraints may wish to remove some of the lines of this file when
    compiling certain programs.

    Modified for Turbo Pascal 5.0

        Copyright 1988, 1990 J.C.Nash
}
{uses Dos, Crt;} {Turbo Pascal 5.0 Modules}
{ 1. Interrupt, Unit, Interface, Implementation, Uses are reserved words now.}
{ 2. System,Dos,Crt are standard unit names in Turbo 5.0.}

const
    big = 1.0E+35;    {a very large number}
    Maxconst = 25;    {Maximum number of constants in data record}
    Maxobs = 100;     {Maximum number of observations in data record}
    Maxparm = 25;     {Maximum number of parameters to adjust}
    Maxvars = 10;     {Maximum number of variables in data record}
    acctol = 0.0001;  {acceptable point tolerance for minimisation codes}
    maxm = 20;        {Maximum number or rows in a matrix}
    maxn = 20;        {Maximum number of columns in a matrix}
    maxmn = 40;       {maxn+maxm, the number of rows in a working array}
    maxsym = 210;     {maximum number of elements of a symmetric matrix
        which need to be stored = maxm * (maxm + 1)/2 }
    reltest = 10.0;   {a relative size used to check equality of numbers.
        Numbers x and y are considered equal if the
        floating-point representation of reltest*x equals
        that of reltest*y.}
    stepredn = 0.2;   {factor to reduce stepsize in line search}
    yearwrit = 1990;  {year in which file was written}

type
    str2 = string[2];
    rmatrix = array[1..maxm, 1..maxn] of real; {a real matrix}
    wmatrix = array[1..maxmn, 1..maxn] of real; {a working array, formed
        as one real matrix stacked on another}
    smatvec = array[1..maxsym] of real; {a vector to store a symmetric matrix
        as the row-wise expansion of its lower triangle}
    rvector = array[1..maxm] of real; {a real vector. We will use vectors
        of m elements always. While this is NOT space efficient,
        it simplifies program codes.}
    cgmethodtype= (Fletcher_Reeves,Polak_Ribiere,Beale_Sorenson);
        {three possible forms of the conjugate gradients updating formulae}
    probdata = record
        m      : integer; {number of observations}
        nvar   : integer; {number of variables}
        nconst: integer; {number of constants}
        vconst: array[1..Maxconst] of real;

```

```

        Ydata : array[1..Maxobs, 1..Maxvars] of real;
        nlls   : boolean; {true if problem is nonlinear least squares}
    end;
{
    NOTE: Pascal does not let us define the work-space for the function
    within the user-defined code. This is a weakness of Pascal for this
    type of work.
}
var {global definitions}
    banner      : string[80]; {program name and description}

function calceps:real;
{calceps.pas ==
    This function returns the machine EPSILON or floating point tolerance,
    the smallest positive real number such that 1.0 + EPSILON > 1.0.
    EPSILON is needed to set various tolerances for different algorithms.
    While it could be entered as a constant, I prefer to calculate it, since
    users tend to move software between machines without paying attention to
    the computing environment. Note that more complete routines exist.
}
var
    e,e0: real;
    i: integer;
begin {calculate machine epsilon}
    e0 := 1; i:=0;
    repeat
        e0 := e0/2; e := 1+e0; i := i+1;
    until (e=1.0) or (i=50); {note safety check}
    e0 := e0*2;
{ Writeln('Machine EPSILON =',e0);}
    calceps:=e0;
end; {calceps}

procedure givens( nRow,nCol : integer;
                  var A, Q: rmatrix);
var
    i, j, k, mn: integer;
    b, c, eps, p, s : real;
begin
    writeln('alg03.pas -- Givens',chr(39),' reduction -- column-wise');
    mn := nRow; if nRow>nCol then mn := nCol;
    for i := 1 to nRow do
        begin
            for j := 1 to nRow do Q[i,j] := 0.0;
            Q[i,i] := 1.0;
        end;
        eps := calceps;
        for j := 1 to (mn-1) do
            begin
                for k := (j+1) to nRow do

```

```

begin
  c := A[j,j]; s := A[k,j];
  b := abs(c); if abs(s)>b then b := abs(s);
  if b>0 then
    begin
      c := c/b; s := s/b;
      p := sqrt(c*c+s*s);
      s := s/p;
      if abs(s)>=eps then
        begin
          c := c/p;
          for i := 1 to nCol do
            begin
              p := A[j,i]; A[j,i] := c*p+s*A[k,i]; A[k,i] := -s*p+c*A[k,i];
            end;
          for i := 1 to nRow do
            begin
              p := Q[i,j]; Q[i,j] := c*p+s*Q[i,k]; Q[i,k] := -s*p+c*Q[i,k];
            end;
          end;
        end;
      end;
    end;
  end;
end;

Procedure Frank2(var m, n: integer; var A: rmatrix);
var
  i,j: integer;
begin
  for i:=1 to m do
    begin
      for j:=1 to n do
        begin
          write(i,' ',j,');
          if (i <= j) then
            A[i,j]:=i
          else
            A[i,j]:=j;
          writeln(A[i,j]);
        end;
      end;
    end;
end;

var
  A, Q: rmatrix;
  i, j, k, nRow, nCol : integer;
  Acopy : rmatrix;
  s : real;

begin
  banner:='dr03.pas -- driver for Givens'+chr(39)+' reduction';

```



```

nRow := 5;
nCol := 3; {Specific to this example.}
writeln('Size of problem (rows, columns)  (' ,nRow,' , ',nCol,')');
writeln('Frank matrix example');
Frank2(nRow, nCol, A);
writeln('Matrix A');
for i:=1 to nRow do
begin
  for j:=1 to nCol do
  begin
    Acopy[i,j]:=A[i,j];
    write(A[i,j]:10:5,' ');
    if (7 * (j div 7) = j) and (j<nCol) then
    begin
      writeln;
    end;
  end;
  writeln;
end;
givens(nRow,nCol,A,Q);
writeln('Decomposition');
writeln('Q');
for i:=1 to nRow do
begin
  for j:=1 to nRow do
  begin
    write(Q[i,j]:10:5,' ');
    if (7 * (j div 7) = j) and (j<nRow) then
    begin
      writeln;
    end;
  end;
  writeln;
end;
writeln('R');
for i:=1 to nRow do
begin
  for j:=1 to nCol do
  begin
    write(A[i,j]:10:5,' ');
    if (7 * (j div 7) = j) and (j<nCol) then
    begin
      writeln;
    end;
  end;
  writeln;
end;
writeln('Q*R - Acopy');
for i:=1 to nRow do
begin
  for j:=1 to nCol do
  begin
    s:=-Acopy[i,j];

```

```

    for k:=1 to nRow do s:=s+Q[i,k]*A[k,j];
    write(s:10,' ');
    if (7 * (j div 7) = j) and (j<nRow) then
    begin
        writeln;
    end;
    end;
    writeln;
end;
end. {dr03.pas == Givens' reduction driver}

```

Example output – column-wise approach

```

fpc ../Pascal2021/dr03.pas
mv ../Pascal2021/dr03 ../Pascal2021/dr03.run
../Pascal2021/dr03.run >../Pascal2021/dr03.out

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr03.pas
## Linking ../Pascal2021/dr03
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 226 lines compiled, 0.1 sec

Size of problem (rows, columns)  (5, 3)
Frank matrix example
1 1; 1.0000000000000000E+000
1 2; 1.0000000000000000E+000
1 3; 1.0000000000000000E+000
2 1; 1.0000000000000000E+000
2 2; 2.0000000000000000E+000
2 3; 2.0000000000000000E+000
3 1; 1.0000000000000000E+000
3 2; 2.0000000000000000E+000
3 3; 3.0000000000000000E+000
4 1; 1.0000000000000000E+000
4 2; 2.0000000000000000E+000
4 3; 3.0000000000000000E+000
5 1; 1.0000000000000000E+000
5 2; 2.0000000000000000E+000
5 3; 3.0000000000000000E+000
Matrix A
  1.00000    1.00000    1.00000
  1.00000    2.00000    2.00000
  1.00000    2.00000    3.00000
  1.00000    2.00000    3.00000
  1.00000    2.00000    3.00000
alg03.pas -- Givens' reduction -- column-wise
Decomposition
Q
  0.44721   -0.89443    0.00000    0.00000    0.00000
  0.44721    0.22361   -0.70711   -0.40825   -0.28868
  0.44721    0.22361    0.70711   -0.40825   -0.28868

```

	0.44721	0.22361	0.00000	0.81650	-0.28868
	0.44721	0.22361	0.00000	0.00000	0.86603
R					
	2.23607	4.02492	5.36656		
	0.00000	0.89443	1.56525		
	0.00000	0.00000	0.70711		
	0.00000	0.00000	0.40825		
	-0.00000	-0.00000	0.28868		
Q*R - Acopy					
	1.45E-016	2.22E-016	6.95E-016		
	1.45E-016	-1.03E-016	-1.11E-016		
	2.81E-016	2.86E-016	2.36E-016		
	-1.26E-016	-4.64E-016	-8.05E-016		
	-2.22E-016	-2.46E-016	-5.00E-016		

Algorithms 5 and 6 – Gaussian elimination and back-solution

Fortran

```
gfortran ../fortran/dr0506.f
mv ./a.out ../fortran/dr0506.run
../fortran/dr0506.run > ../fortran/dr0506out.txt

ORDER= 4 ORIGINAL MATRIX WITH RHS APPENDED
ROW 1
  1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 4.00000E+00
ROW 2
  1.00000E+00 2.00000E+00 2.00000E+00 2.00000E+00 7.00000E+00
ROW 3
  1.00000E+00 2.00000E+00 3.00000E+00 3.00000E+00 9.00000E+00
ROW 4
  1.00000E+00 2.00000E+00 3.00000E+00 4.00000E+00 1.00000E+01
DETERMINANT= 1.00000E+00
SOLN X( 1)= 1.00000E+00 ERROR= 0.00000E+00
SOLN X( 2)= 1.00000E+00 ERROR= 0.00000E+00
SOLN X( 3)= 1.00000E+00 ERROR= 0.00000E+00
SOLN X( 4)= 1.00000E+00 ERROR= 0.00000E+00
ORDER= 8 ORIGINAL MATRIX WITH RHS APPENDED
ROW 1
  1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00
  1.00000E+00 1.00000E+00 1.00000E+00 8.00000E+00
ROW 2
  1.00000E+00 2.00000E+00 2.00000E+00 2.00000E+00 2.00000E+00
  2.00000E+00 2.00000E+00 2.00000E+00 1.50000E+01
ROW 3
  1.00000E+00 2.00000E+00 3.00000E+00 3.00000E+00 3.00000E+00
  3.00000E+00 3.00000E+00 3.00000E+00 2.10000E+01
ROW 4
  1.00000E+00 2.00000E+00 3.00000E+00 4.00000E+00 4.00000E+00
  4.00000E+00 4.00000E+00 4.00000E+00 2.60000E+01
ROW 5
  1.00000E+00 2.00000E+00 3.00000E+00 4.00000E+00 5.00000E+00
  5.00000E+00 5.00000E+00 5.00000E+00 3.00000E+01
ROW 6
  1.00000E+00 2.00000E+00 3.00000E+00 4.00000E+00 5.00000E+00
  6.00000E+00 6.00000E+00 6.00000E+00 3.30000E+01
ROW 7
  1.00000E+00 2.00000E+00 3.00000E+00 4.00000E+00 5.00000E+00
  6.00000E+00 7.00000E+00 7.00000E+00 3.50000E+01
ROW 8
  1.00000E+00 2.00000E+00 3.00000E+00 4.00000E+00 5.00000E+00
  6.00000E+00 7.00000E+00 8.00000E+00 3.60000E+01
DETERMINANT= 1.00000E+00
SOLN X( 1)= 1.00000E+00 ERROR= 0.00000E+00
SOLN X( 2)= 1.00000E+00 ERROR= 0.00000E+00
SOLN X( 3)= 1.00000E+00 ERROR= 0.00000E+00
SOLN X( 4)= 1.00000E+00 ERROR= 0.00000E+00
SOLN X( 5)= 1.00000E+00 ERROR= 0.00000E+00
SOLN X( 6)= 1.00000E+00 ERROR= 0.00000E+00
```

```
SOLN X( 7)= 1.00000E+00   ERROR= 0.00000E+00
SOLN X( 8)= 1.00000E+00   ERROR= 0.00000E+00
```

Pascal

Listing – column-wise approach

```
program givrun(input, output);
{dr03.PAS == driver for Givens' reduction of a matrix

    Copyright 1988 J.C.Nash
}
{I constype.def}
{constype.def ==
    This file contains various definitions and type statements which are
    used throughout the collection of "Compact Numerical Methods". In many
    cases not all definitions are needed, and users with very tight memory
    constraints may wish to remove some of the lines of this file when
    compiling certain programs.

    Modified for Turbo Pascal 5.0

    Copyright 1988, 1990 J.C.Nash
}
{uses Dos, Crt;} {Turbo Pascal 5.0 Modules}
{ 1. Interrupt, Unit, Interface, Implementation, Uses are reserved words now.}
{ 2. System,Dos,Crt are standard unit names in Turbo 5.0.}

const
    big = 1.0E+35;    {a very large number}
    Maxconst = 25;    {Maximum number of constants in data record}
    Maxobs = 100;     {Maximum number of observations in data record}
    Maxparm = 25;     {Maximum number of parameters to adjust}
    Maxvars = 10;     {Maximum number of variables in data record}
    acctol = 0.0001;  {acceptable point tolerance for minimisation codes}
    maxm = 20;        {Maximum number or rows in a matrix}
    maxn = 20;        {Maximum number of columns in a matrix}
    maxmn = 40;       {maxn+maxm, the number of rows in a working array}
    maxsym = 210;     {maximum number of elements of a symmetric matrix
        which need to be stored = maxm * (maxm + 1)/2 }
    reltest = 10.0;   {a relative size used to check equality of numbers.
        Numbers x and y are considered equal if the
        floating-point representation of reltest+x equals
        that of reltest+y.}
    stepredn = 0.2;   {factor to reduce stepsize in line search}
    yearwrit = 1990;  {year in which file was written}

type
    str2 = string[2];
    rmatrix = array[1..maxm, 1..maxn] of real; {a real matrix}
    wmatrix = array[1..maxmn, 1..maxn] of real; {a working array, formed
        as one real matrix stacked on another}
    smatvec = array[1..maxsym] of real; {a vector to store a symmetric matrix
```

```

        as the row-wise expansion of its lower triangle}
rvector = array[1..maxm] of real; {a real vector. We will use vectors
    of m elements always. While this is NOT space efficient,
    it simplifies program codes.}
cgmethodtype= (Fletcher_Reeves,Polak_Ribiere,Beale_Sorenson);
    {three possible forms of the conjugate gradients updating formulae}
probddata = record
    m      : integer; {number of observations}
    nvar   : integer; {number of variables}
    nconst: integer; {number of constants}
    vconst: array[1..Maxconst] of real;
    Ydata  : array[1..Maxobs, 1..Maxvars] of real;
    nlls   : boolean; {true if problem is nonlinear least squares}
end;

{
NOTE: Pascal does not let us define the work-space for the function
within the user-defined code. This is a weakness of Pascal for this
type of work.
}
var {global definitions}
    banner      : string[80]; {program name and description}

function calceps:real;
{calceps.pas ==
    This function returns the machine EPSILON or floating point tolerance,
    the smallest positive real number such that 1.0 + EPSILON > 1.0.
    EPSILON is needed to set various tolerances for different algorithms.
    While it could be entered as a constant, I prefer to calculate it, since
    users tend to move software between machines without paying attention to
    the computing environment. Note that more complete routines exist.
}
var
    e,e0: real;
    i: integer;
begin {calculate machine epsilon}
    e0 := 1; i:=0;
    repeat
        e0 := e0/2; e := 1+e0; i := i+1;
    until (e=1.0) or (i=50); {note safety check}
    e0 := e0*2;
{ Writeln('Machine EPSILON =',e0);}
    calceps:=e0;
end; {calceps}

procedure givens( nRow,nCol : integer;
                 var A, Q: rmatrix);
var
    i, j, k, mn: integer;
    b, c, eps, p, s : real;
begin

```

```

writeln('alg03.pas -- Givens',chr(39),' reduction -- column-wise');
mn := nRow; if nRow>nCol then mn := nCol;
for i := 1 to nRow do
begin
  for j := 1 to nRow do Q[i,j] := 0.0;
  Q[i,i] := 1.0;
end;
eps := calceps;
for j := 1 to (mn-1) do
begin
  for k := (j+1) to nRow do
  begin
    c := A[j,j]; s := A[k,j];
    b := abs(c); if abs(s)>b then b := abs(s);
    if b>0 then
    begin
      c := c/b; s := s/b;
      p := sqrt(c*c+s*s);
      s := s/p;
      if abs(s)>=eps then
      begin
        c := c/p;
        for i := 1 to nCol do
        begin
          p := A[j,i]; A[j,i] := c*p+s*A[k,i]; A[k,i] := -s*p+c*A[k,i];
        end;
        for i := 1 to nRow do
        begin
          p := Q[i,j]; Q[i,j] := c*p+s*Q[i,k]; Q[i,k] := -s*p+c*Q[i,k];
        end;
      end;
    end;
  end;
end;
end;
end;

Procedure Frank2(var m, n: integer; var A: rmatrix);
var
  i,j: integer;
begin
  for i:=1 to m do
  begin
    for j:=1 to n do
    begin
      write(i, ' ',j,');
      if (i <= j) then
        A[i,j]:=i
      else
        A[i,j]:=j;
      writeln(A[i,j]);
    end;
  end;
end;

```

```

var
  A, Q: rmatrix;
  i, j, k, nRow, nCol : integer;
  Acopy : rmatrix;
  s : real;

begin
  banner:='dr03.pas -- driver for Givens'+chr(39)+' reduction';
  nRow := 5;
  nCol := 3; {Specific to this example.}
  writeln('Size of problem (rows, columns)  ('',nRow,', ', '',nCol,'')');
  writeln('Frank matrix example');
  Frank2(nRow, nCol, A);
  writeln('Matrix A');
  for i:=1 to nRow do
  begin
    for j:=1 to nCol do
    begin
      Acopy[i,j]:=A[i,j];
      write(A[i,j]:10:5, ' ');
      if (7 * (j div 7) = j) and (j<nCol) then
      begin
        writeln;
      end;
    end;
    writeln;
  end;
  givens(nRow,nCol,A,Q);
  writeln('Decomposition');
  writeln('Q');
  for i:=1 to nRow do
  begin
    for j:=1 to nRow do
    begin
      write(Q[i,j]:10:5, ' ');
      if (7 * (j div 7) = j) and (j<nRow) then
      begin
        writeln;
      end;
    end;
    writeln;
  end;
  writeln('R');
  for i:=1 to nRow do
  begin
    for j:=1 to nCol do
    begin
      write(A[i,j]:10:5, ' ');
      if (7 * (j div 7) = j) and (j<nCol) then
      begin
        writeln;
      end;
    end;
  end;
end;

```



```

        end;
    end;
    writeln;
end;
writeln('Q*R - Acopy');
for i:=1 to nRow do
begin
    for j:=1 to nCol do
    begin
        s:=-Acopy[i,j];
        for k:=1 to nRow do s:=s+Q[i,k]*A[k,j];
        write(s:10,' ');
        if (7 * (j div 7) = j) and (j<nRow) then
        begin
            writeln;
        end;
    end;
    writeln;
end;
end. {dr03.pas == Givens' reduction driver}

```

Example output – column-wise approach

```

fpc ../Pascal2021/dr0506.pas
mv ../Pascal2021/dr0506 ../Pascal2021/dr0506.run
../Pascal2021/dr0506.run >../Pascal2021/dr0506.out

```

```

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr0506.pas
## Linking ../Pascal2021/dr0506
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 257 lines compiled, 0.1 sec

```

Data matrix :4 by 5

```

Row 1
  1.00000    2.00000    3.00000    4.00000   10.00000
Row 2
  2.00000    2.00000    3.00000    4.00000   11.00000
Row 3
  3.00000    3.00000    3.00000    4.00000   13.00000
Row 4
  4.00000    4.00000    4.00000    4.00000   16.00000

```

tol for pivot = 2.8421709430404007E-014

alg05.pas -- Gauss elimination with partial pivoting

Interchanging rows 4 and 1

Interchanging rows 4 and 2

Interchanging rows 4 and 3

Gauss elimination complete -- determinant = -2.4000000000000000E+001

returned matrix 4 by 5

```

Row 1
  4.00000    4.00000    4.00000    4.00000   16.00000 Row 2

```

```

0.50000    1.00000    2.00000    3.00000    6.00000 Row 3
0.75000    0.00000    1.00000    2.00000    3.00000 Row 4
0.25000    0.00000    0.00000    1.00000    1.00000
alg06.pas -- Gauss elimination back-substitution
Solution 1
1.00000    1.00000    1.00000    1.00000
Residuals
0.00E+000  0.00E+000  0.00E+000  0.00E+000
Sum of squared residuals = 0.000000000000000E+000
Data matrix :8 by 9
Row 1
1.00000    2.00000    3.00000    4.00000    5.00000    6.00000    7.00000
8.00000    36.00000
Row 2
2.00000    2.00000    3.00000    4.00000    5.00000    6.00000    7.00000
8.00000    37.00000
Row 3
3.00000    3.00000    3.00000    4.00000    5.00000    6.00000    7.00000
8.00000    39.00000
Row 4
4.00000    4.00000    4.00000    4.00000    5.00000    6.00000    7.00000
8.00000    42.00000
Row 5
5.00000    5.00000    5.00000    5.00000    5.00000    6.00000    7.00000
8.00000    46.00000
Row 6
6.00000    6.00000    6.00000    6.00000    6.00000    6.00000    7.00000
8.00000    51.00000
Row 7
7.00000    7.00000    7.00000    7.00000    7.00000    7.00000    7.00000
8.00000    57.00000
Row 8
8.00000    8.00000    8.00000    8.00000    8.00000    8.00000    8.00000
8.00000    64.00000

tol for pivod = 1.1368683772161603E-013
alg05.pas -- Gauss elimination with partial pivoting
Interchanging rows 8 and 1
Interchanging rows 8 and 2
Interchanging rows 8 and 3
Interchanging rows 8 and 4
Interchanging rows 8 and 5
Interchanging rows 8 and 6
Interchanging rows 8 and 7
Gauss elimination complete -- determinant = -4.032000000000000E+004
returned matrix 8 by 9
Row 1
8.00000    8.00000    8.00000    8.00000    8.00000    8.00000    8.00000
8.00000    64.00000 Row 2
0.25000    1.00000    2.00000    3.00000    4.00000    5.00000    6.00000
7.00000    28.00000 Row 3
0.37500    0.00000    1.00000    2.00000    3.00000    4.00000    5.00000
6.00000    21.00000 Row 4

```

```

0.50000  0.00000  0.00000  1.00000  2.00000  3.00000  4.00000
5.00000  15.00000 Row 5
0.62500  0.00000  0.00000  0.00000  1.00000  2.00000  3.00000
4.00000  10.00000 Row 6
0.75000  0.00000  0.00000  0.00000  0.00000  1.00000  2.00000
3.00000  6.00000 Row 7
0.87500  0.00000  0.00000  0.00000  0.00000  0.00000  1.00000
2.00000  3.00000 Row 8
0.12500  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
1.00000  1.00000
alg06.pas -- Gauss elimination back-substitution
Solution 1
1.00000  1.00000  1.00000  1.00000  1.00000  1.00000  1.00000
1.00000
Residuals
0.00E+000  0.00E+000  0.00E+000  0.00E+000  0.00E+000  0.00E+000  0.00E+000
0.00E+000
Sum of squared residuals = 0.0000000000000000E+000

```

Algorithm 9 – Bauer-Reinsch matrix inversion

Wilkinson, Reinsch, and Bauer (1971), pages 45-49, is a contribution entitled **Inversion of Positive Definite Matrices by the Gauss-Jordan Method**. It hardly mentions, but appears to assume, that the matrix to be inverted is symmetric. Two Algol procedures are provided, one for a matrix stored as a square array, the other for the a matrix where only the lower triangle is stored as a single vector in row-wise order. That is, if A is of order $n=3$ and has values

```
1  2  4
2  3  5
4  5  6
```

Then the corresponding vector of $6 = n*(n+1)/2$ values is

```
1  2  3  4  5  6
```

By some exceedingly clever coding and matrix manipulation, Bauer and Reinsch developed tiny codes that invert a positive-definite matrix *in situ* using only one extra vector of length n . Thus, besides the memory to store a very small code, we need only $n*(n+3)/2$ floating point numbers and a few integers to index arrays.

Truthfully, we rarely need an explicit matrix inverse, and the most common positive-definite symmetric matrix that arises in scientific computations is the sum of squares and cross-products (SSCP) in the normal equations used for linear (or also nonlinear) least squares problems. However, the formation of this SSCP matrix is rarely the best approach to solving least squares problems. The SVD introduced in Algorithm 1 and the least squares solution in Algorithm 2 lead to better methods. (??mention A4, Choleski in A7, A8 etc.)

Despite these caveats, the Bauer-Reinsch algorithm is interesting as a historical curiosity, showing what can be done when resources are very limited.

Fortran

Listing

```
C&&& A9
C TEST ALGORITHM 9 A9GJ
C J.C. NASH JULY 1978, APRIL 1989
C USE FRANK MATRIX
  LOGICAL INDEF
  INTEGER N,N2,I,J,IJ,NOUT
  REAL A(55),X(10),S,T
  N2=55
C PRINTER CHANNEL
  NOUT=6
C MAIN LOOP
C DO 100 N=2,10,2
  N = 4
  WRITE(NOUT,950)N
950 FORMAT('OORDER=',I4,' ORIGINAL MATRIX')
C PUT IN CARDS FROM A78
C NOTE DIFFERENCES ONLY IN CALLS
  DO 20 I=1,N
    DO 10 J=1,I
      IJ=I*(I-1)/2+J
      A(IJ)=J
10    CONTINUE
20    CONTINUE
  CALL SOUT(A,N2,N,NOUT)
```

```

        CALL A9GJ(A,N2,N,INDEF,X)
        WRITE(NOUT,956)
956    FORMAT('OINVERSE')
        CALL SOUT(A,N2,N,NOUT)
        WRITE(NOUT,957)
957    FORMAT('OINVERSE OF INVERSE')
        CALL A9GJ(A,N2,N,INDEF,X)
        CALL SOUT(A,N2,N,NOUT)
C     COMPUTE DEVIATION FROM ORIGINAL MATRIX
        S=0.0
        DO 50 I=1,N
            DO 40 J=1,I
                IJ=I*(I-1)/2+J
                T=ABS(J-A(IJ))
                IF(T.GT.S)S=T
40        CONTINUE
50    CONTINUE
        WRITE(NOUT,958)S
958    FORMAT('OMAX. DEVN. OF INVERSE-INVERSE FROM ORIGINAL=',1PE16.8)
C 100 CONTINUE
        STOP
        END
        SUBROUTINE SOUT(A,N2,N,NOUT)
C   J.C. NASH    JULY 1978, APRIL 1989
        INTEGER N2,N,NOUT,I,J,IJ,JJ
        REAL A(N2)
C     PRINTS SYMMETRIC MATRIX STORED ROW-WISE AS A VECTOR
        DO 20 I=1,N
            WRITE(NOUT,951)I
951    FORMAT(' ROW',I3)
            IJ=I*(I-1)/2+1
            JJ=IJ+I-1
            WRITE(NOUT,952)(A(J),J=IJ,JJ)
952    FORMAT(1H ,1P5E16.8)
20    CONTINUE
        RETURN
        END
        SUBROUTINE A9GJ(A,N2,N,INDEF,X)
C   ALGORITHM 9
C   J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C   BAUER-REINSCH GAUSS-JORDAN INVERSION OF A SYMMETRIC, POSITIVE
C   A=MATRIX - STORED AS A VECTOR -- ELEMENT I,J IN POSITION I*(I-1)/2+J
C   N2=LENGTH OF VECTOR A = N*(N+1)/2
C   N=ORDER OF MATRIX
C   INDEF=LOGICAL FLAG SET .TRUE. IF MATRIX NOT COMPUTATIONALLY
C   POSITIVE DEFINITE
C   X=WORKING VECTOR OF LENGTH AT LEAST N
C   DEFINITE MATRIX
C   STEP 0
        LOGICAL INDEF
        INTEGER N2,N,K,KK,Q,M,Q2,JI,JQ
        REAL A(N2),S,T,X(N)
C   STEP 1

```

```

        INDEF=.FALSE.
        DO 100 KK=1,N
            K=N+1-KK
C   STEP 2
            S=A(1)
C   STEP 3
            IF(S.LE.0.0) INDEF=.TRUE.
            IF(INDEF) RETURN
C   STEP 4
            M=1
C   STEP 5
            DO 60 I=2,N
C   STEP 6
                Q=M
                M=M+I
                T=A(Q+1)
                X(I)=-T/S
C   STEP 7
                Q2=Q+2
                IF(I.GT.K) X(I)=-X(I)
C   STEP 8
                DO 40 J=Q2,M
                    JI=J-I
                    JQ=J-Q
                    A(JI)=A(J)+T*X(JQ)
40             CONTINUE
C   STEP 9
60             CONTINUE
C   STEP 10
                Q=Q-1
                A(M)=1/S
C   STEP 11
                DO 80 I=2,N
                    JI=Q+I
                    A(JI)=X(I)
80             CONTINUE
C   STEP 12
100            CONTINUE
                RETURN
            END

```

Example output

```

## #!/bin/bash
gfortran ../fortran/a9.f
mv ./a.out ../fortran/a9.run
../fortran/a9.run

## OORDER=    4  ORIGINAL MATRIX
## ROW  1
##    1.00000000E+00
## ROW  2
##    1.00000000E+00  2.00000000E+00
## ROW  3

```

```

##      1.00000000E+00  2.00000000E+00  3.00000000E+00
## ROW  4
##      1.00000000E+00  2.00000000E+00  3.00000000E+00  4.00000000E+00
## OINVERSE
## ROW  1
##      2.00000000E+00
## ROW  2
##     -1.00000000E+00  2.00000000E+00
## ROW  3
##      0.00000000E+00 -1.00000000E+00  2.00000000E+00
## ROW  4
##      0.00000000E+00  0.00000000E+00 -1.00000000E+00  1.00000000E+00
## OINVERSE OF INVERSE
## ROW  1
##      1.00000012E+00
## ROW  2
##      1.00000024E+00  2.00000048E+00
## ROW  3
##      1.00000036E+00  2.00000072E+00  3.00000095E+00
## ROW  4
##      1.00000036E+00  2.00000072E+00  3.00000095E+00  4.00000095E+00
## OMAX. DEVN. OF INVERSE-INVERSE FROM ORIGINAL=  9.53674316E-07

```

BASIC

Listing

```

10 PRINT "ALGORITHM 9 - BAUER REINSCH INVERSION TEST"
20 N=100
40 DIM A(N*(N+1)/2),X(N)
45 LET N=4
50 GOSUB 1500
51 REM BUILD MATRIX IN A
60 GOSUB 1400
61 REM PRINT IT
70 GOSUB 1000
71 REM INVERT
80 GOSUB 1400
81 REM PRINT
90 quit
110 STOP
1000 REM ALG. 9 BAUER REINSCH INVERSION
1010 FOR K=N TO 1 STEP -1
1011     REM STEP 1
1020     S=A(1)
1021     REM STEP 2
1030     IF S<=0 THEN EXIT 1160
1031     REM STEP 3
1040     M=1
1041     REM STEP 4
1050     FOR I=2 TO N
1051         REM STEP 5
1060         Q=M
1061         M=M+I

```

```

1062     T=A(Q+1)
1063     X(I)=-T/S
1064     REM STEP 6
1070     IF I>K THEN X(I)=-X(I)
1071     REM STEP 7
1080     FOR J=Q+2 TO M
1081     REM STEP 8
1090         A(J-I)=A(J)+T*X(J-Q)
1100     NEXT J
1110 NEXT I
1111     REM STEP 9
1120     Q=Q-1
1121     A(M)=1/S
1122     REM STEP 10
1130     FOR I=2 TO N
1131         A(Q+I)=X(I)
1132     NEXT I
1133     REM STEP 11
1140 NEXT K
1141     REM STEP 12
1150 RETURN
1160 PRINT "MATRIX COMPUTATIONALLY INDEFINITE"
1170 STOP
1171     REM END ALG. 9
1400 PRINT "MATRIX A"
1410 FOR I=1 TO N
1420 FOR J=1 TO I
1430 PRINT A(I*(I-1)/2+J);
1440 NEXT J
1450 PRINT
1460 NEXT I
1470 RETURN
1500 REM FRANK MATRIX
1510 FOR I=1 TO N
1520 FOR J=1 TO I
1530 LET A(I*(I-1)/2+J)=J
1540 NEXT J
1550 NEXT I
1560 RETURN

```

Example output

```

bwbasic ../BASIC/a9.bas >../BASIC/a9.out
# echo "done"

```

Bywater BASIC Interpreter/Shell, version 2.20 patch level 2

Copyright (c) 1993, Ted A. Campbell

Copyright (c) 1995-1997, Jon B. Volkoff

ALGORITHM 9 - BAUER REINSCH INVERSION TEST


```

MATRIX A
1
1 2
1 2 3
1 2 3 4
MATRIX A
2
-1 2
0 -1 2
0 0 -1 1

```

Pascal

Listing

```

program dr09(input,output);
{dr09.pas == driver program to test procedure for the Bauer-Reinsch
  inversion of a symmetric positive definite real matrix stored
  in row-wise vector form

  Copyright 1988 J.C.Nash
}
{I constype.def}
{constype.def ==
  This file contains various definitions and type statements which are
  used throughout the collection of "Compact Numerical Methods". In many
  cases not all definitions are needed, and users with very tight memory
  constraints may wish to remove some of the lines of this file when
  compiling certain programs.

  Modified for Turbo Pascal 5.0

  Copyright 1988, 1990 J.C.Nash
}
{uses Dos, Crt;} {Turbo Pascal 5.0 Modules}
{ 1. Interrupt, Unit, Interface, Implementation, Uses are reserved words now.}
{ 2. System,Dos,Crt are standard unit names in Turbo 5.0.}

const
  big = 1.0E+35;    {a very large number}
  Maxconst = 25;    {Maximum number of constants in data record}
  Maxobs = 100;     {Maximum number of observations in data record}
  Maxparm = 25;     {Maximum number of parameters to adjust}
  Maxvars = 10;     {Maximum number of variables in data record}
  acctol = 0.0001;  {acceptable point tolerance for minimisation codes}
  maxm = 20;        {Maximum number or rows in a matrix}
  maxn = 20;        {Maximum number of columns in a matrix}
  maxmn = 40;       {maxn+maxm, the number of rows in a working array}
  maxsym = 210;     {maximum number of elements of a symmetric matrix
                    which need to be stored = maxm * (maxm + 1)/2 }
  reltest = 10.0;   {a relative size used to check equality of numbers.
                    Numbers x and y are considered equal if the
                    floating-point representation of reltest*x equals

```

```

        that of reltest+y.)
stepredn = 0.2;    {factor to reduce stepsize in line search}
yearwrit = 1990;  {year in which file was written}

type
  str2 = string[2];
  rmatrix = array[1..maxm, 1..maxn] of real; {a real matrix}
  wmatrix = array[1..maxmn, 1..maxn] of real; {a working array, formed
        as one real matrix stacked on another}
  smatvec = array[1..maxsym] of real; {a vector to store a symmetric matrix
        as the row-wise expansion of its lower triangle}
  rvector = array[1..maxm] of real; {a real vector. We will use vectors
        of m elements always. While this is NOT space efficient,
        it simplifies program codes.}
  cgmethodtype= (Fletcher_Reeves,Polak_Ribiere,Beale_Sorenson);
  {three possible forms of the conjugate gradients updating formulae}
  probdata = record
    m      : integer; {number of observations}
    nvar   : integer; {number of variables}
    nconst : integer; {number of constants}
    vconst : array[1..Maxconst] of real;
    Ydata  : array[1..Maxobs, 1..Maxvars] of real;
    nlls   : boolean; {true if problem is nonlinear least squares}
  end;

{
  NOTE: Pascal does not let us define the work-space for the function
  within the user-defined code. This is a weakness of Pascal for this
  type of work.
}
var {global definitions}
  banner      : string[80]; {program name and description}

Procedure Frank(var n: integer; var A: rmatrix; var avector: smatvec);
var
  i,j: integer;
begin
  writeln('Frank symmetric');
  for i:=1 to n do
    begin
      for j:=1 to i do
        begin
          A[i,j]:=j;
          A[j,i]:=j;
        end;
      end;
    end;
end;

Procedure mat2vec(var n: integer; var A: rmatrix; var avector: smatvec);
var
  i,j,k: integer;

begin {convert to vector form}
  k:=0; {index for vector element}

```

```

    for i:=1 to n do
    begin
        for j:=1 to i do
        begin
            k:=k+1;
            avector[k]:=A[i,j];
        end;
    end;
end; {matrixin}

Procedure vec2mat(var n: integer; var A: rmatrix; var avector: smatvec);
var
    i,j,k: integer;

begin {convert to matrix form}
    k:=0; {index for vector element}
    for i:=1 to n do
    begin
        for j:=1 to i do
        begin
            k:=k+1;
            A[i,j]:=avector[k];
        end;
    end;
end; {matrixin}

{ I alg09.pas}
procedure brspdmi(n : integer;
                 var avector : smatvec;
                 var singmat : boolean);

var
    i,j,k,m,q : integer;
    s,t : real;
    X : rvector;

begin
    writeln('alg09.pas -- Bauer Reinsch inversion');
    singmat := false;
    for k := n downto 1 do
    begin
        if (not singmat) then
        begin
            s := avector[1];
            if s>0.0 then
            begin
                m := 1;
                for i := 2 to n do
                begin
                    q := m; m := m+i; t := avector[q+1]; X[i] := -t/s;

                    if i>k then X[i] := -X[i];
                    for j := (q+2) to m do

```

```

        begin
            avector[j-i] := avector[j]+t*X[j-q];
        end;
    end;
    q := q-1; avector[m] := 1.0/s;
    for i := 2 to n do avector[q+i] := X[i];
end
else
    singmat := true;
end;
end;
end;
end;

var
    A, Ainverse : rmatrix;
    avector : smatvec;
    i, imax, j, jmax, k, n : integer;
    errmax, s : real;
    singmat: boolean;

BEGIN { main program }
    banner:='dr09.pas -- test Bauer Reinsch sym, posdef matrix inversion';
    writeln(banner);
    n:=4; {Fixed example size 20210113}
    Frank(n,A,avector);
    writeln;
    writeln('returned matrix of order ',n);
    begin
        for i:=1 to n do
            begin
                for j:=1 to n do
                    begin
                        write(A[i,j], ' ');
                    end;
                    writeln;
                end;
            end;
        end;
    end;
    mat2vec(n, A, avector);
    begin
        writeln('Symmetric matrix -- Vector form');
        k := 0;
        for i := 1 to n do
            begin
                for j := 1 to i do
                    begin
                        k := k+1;
                        write(avector[k]:10:5, ' ');
                    end;
                    writeln;
                end;
            end;
        end;
    end;
    brspdmi(n, avector,singmat);

```

```

if singmat then halt; {safety check}
writeln('Computed inverse');
k := 0; {initialize index to smatvec elements}
for i := 1 to n do
begin
  for j := 1 to i do
  begin
    k := k+1;
    write(avector[k]:10:5, ' ');
    Ainverse[i,j] := avector[k]; {save square form of inverse}
    Ainverse[j,i] := avector[k];
    if (7 * (j div 7) = j) and (j<i) then
    begin
      writeln;
    end;
  end;
  writeln;
end;
{Compute maximum error in A * Ainverse and note where it occurs.}
errmax := 0.0; imax := 0; jmax := 0;
for i := 1 to n do
begin
  for j := 1 to n do
  begin
    s := 0.0; if i=j then s := -1.0;
    for k := 1 to n do s := s + Ainverse[i,k]*A[k,j];
    {Note: A has not been altered, since avector was used.}
    if abs(s)>abs(errmax) then
    begin
      errmax := s; imax := i; jmax := j; {save maximum error, indices}
    end;
  end; {loop on j}
end; {loop on i}
writeln('Maximum element in Ainverse * A - 1(n) = ',errmax,
        ' position ',imax,',',jmax);
end. {dr09.pas == Bauer Reinsch inversion}

```

Example output

```

fpc ../Pascal2021/dr09.pas
# copy to run file
mv ../Pascal2021/dr09 ../Pascal2021/dr09.run
../Pascal2021/dr09.run >../Pascal2021/dr09p.out

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr09.pas
## Linking ../Pascal2021/dr09
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 233 lines compiled, 0.1 sec

dr09.pas -- test Bauer Reinsch sym, posdef matrix inversion
Frank symmetric

```

```

returned matrix of order 4
1.0000000000000000E+000  1.0000000000000000E+000  1.0000000000000000E+000  1.0000000000000000E+000
1.0000000000000000E+000  2.0000000000000000E+000  2.0000000000000000E+000  2.0000000000000000E+000
1.0000000000000000E+000  2.0000000000000000E+000  3.0000000000000000E+000  3.0000000000000000E+000
1.0000000000000000E+000  2.0000000000000000E+000  3.0000000000000000E+000  4.0000000000000000E+000
Symmetric matrix -- Vector form
1.00000
1.00000  2.00000
1.00000  2.00000  3.00000
1.00000  2.00000  3.00000  4.00000
alg09.pas -- Bauer Reinsch inversion
Computed inverse
2.00000
-1.00000  2.00000
0.00000 -1.00000  2.00000
0.00000  0.00000 -1.00000  1.00000
Maximum element in Ainverse * A - 1(n) = 0.0000000000000000E+000 position 0,0

```

Python

WARNING: interim test only!!!!???

Listing

The Algorithm 9 code:

```

# -*- coding: utf-8 -*-
"""
CNM Algorithm 09 test

J C Nash 2021-1-12
"""

import numpy
import math
import sys
def brspdmi(Avec, n):
# =====
# Bauer Reinsch inverse of symmetric positive definite matrix stored
# as a vector that has the lower triangle of the matrix in row order
# =====
    print(Avec)
    X = numpy.array([ 0 ] * n) # zero vector x
    for k in range(n, 0, -1):
        s = Avec[k];
        #print("s=",s)
        if (s > 0.0) :
            m = 1;
            for i in range(2,n+1):
                q = m
                m = m+i
                t = Avec[q]
                X[i-1] = -t/s
            if i>k :

```

```

        X[i-1] = -X[i-1]
    #     print("i, q, m:", i, q, m)
    for j in range((q+2), m+1):
    #         print(j)
    #         print("j-q-1=", j-q-1)
    #         print(X[j-q-1])
        Avec[j-i-1] = Avec[j-1]+t*X[j-q-1]
    q = q-1
    Avec[m-1] = 1.0/s
    for i in range(2, n+1):
        print("i ",i)
        Avec[q+i-1] = X[i-1]
    else :
        print("Matrix is singular")
        sys.exit()
    print(k,":",Avec)
    return(Avec)

def FrankMat(n):
    Amat = numpy.array([ [ 0 ] * n ] * n) # numpy.empty(shape=(n,n), dtype='object')
    for i in range(1,n+1):
    #         print("i=",i)
        for j in range(1,i+1):
    #             print(j)
            Amat[i-1,j-1]=j
            Amat[j-1,i-1]=j
    return(Amat)

def smat2vec(Amat):
    n=len(Amat[0])
    n2=int(n*(n+1)/2)
    svec = [ None ] * n2
    k = 0
    for i in range(1,n+1):
        for j in range(1,i+1):
            svec[k]=Amat[i-1, j-1]
            k=k+1
    return(svec)

def svec2mat(svec):
    n2=len(svec)
    n=int((-1+math.sqrt(1+8*n2))/2)
    print("matrix is of size ",n)
    Amat = numpy.array([ [ None ] * n ] * n)
    k = 0
    for i in range(1,n+1):
        for j in range(1,i+1):
            Amat[i-1, j-1] = svec[k]
            Amat[j-1, i-1] = svec[k]
            k=k+1
    return(Amat)

# Main program

```

```

AA = FrankMat(4)
print(AA)
avec = smat2vec(AA)
print(avec)
n=len(AA[0])
vinv = brspdmi(avec, n)
## Computed inverse
##      2.00000
##    -1.00000    2.00000
##      0.00000    -1.00000    2.00000
##      0.00000    0.00000   -1.00000    1.00000

print(vinv)
Ainv = svec2mat(vinv)
print(Ainv)
print(AA)
print(numpy.dot(Ainv, AA))

```

Example output

```

python3 ../python/A9.py

## [[1 1 1 1]
##  [1 2 2 2]
##  [1 2 3 3]
##  [1 2 3 4]]
## [1, 1, 2, 1, 2, 3, 1, 2, 3, 4]
## [1, 1, 2, 1, 2, 3, 1, 2, 3, 4]
## i  2
## i  3
## i  4
## 4 : [1, 1, 2, 1, 2, 3, -1, -1, -1, 1.0]
## i  2
## i  3
## i  4
## 3 : [1, 1, 2, 0, 0, 2.0, -1, -1, -1, 1.0]
## i  2
## i  3
## i  4
## 2 : [1, 0, 2.0, 0, -1, 2.0, -1, 0, -1, 1.0]
## i  2
## i  3
## i  4
## 1 : [2.0, -1, 2.0, 0, -1, 2.0, 0, 0, -1, 1.0]
## [2.0, -1, 2.0, 0, -1, 2.0, 0, 0, -1, 1.0]
## matrix is of size 4
## [[2.0 -1 0 0]
##  [-1 2.0 -1 0]
##  [0 -1 2.0 -1]
##  [0 0 -1 1.0]]
## [[1 1 1 1]

```



```
## [1 2 2 2]
## [1 2 3 3]
## [1 2 3 4]]
## [[1.0 0.0 0.0 0.0]
## [0.0 1.0 0.0 0.0]
## [0.0 0.0 1.0 0.0]
## [0.0 0.0 0.0 1.0]]
```

R

Listing and Example output

```
A9 <- function(a, n){
  x <- rep(0, n)
  for (k in n:1){
    s=a[1]
    if (s <= 0){
      stop("A9: matrix is singular")
    }
    m<-1
    for (i in 2:n){
      q<-m; m<-m+i; t<-a[q+1]; x[i]<--t/s
      if (i > k) { x[i] <- -x[i]}
      for (j in (q+2):m){
        a[j-i]<-a[j]+t*x[j-q]
      }
    }
    q<-q-1; a[m]=1/s
    for (i in 2:n){a[q+i] <- x[i]}
  }
  # cat("iteration k:")
  # print(a)
  a
}

FrankMat <- function(n){
  Amat <- matrix(0, nrow=n, ncol=n)
  for (i in 1:n){
    for (j in 1:i){
      Amat[i,j]<-j; Amat[j,i]<-j
    }
  }
  Amat
}

smat2vec <- function(Amat){
  n<-dim(Amat)[1]
  n2<-(n*(n+1))/2
  svec = rep(0, n2)
  k <- 0
  for (i in 1:n){
    for (j in 1:i){
      k<-k+1
      svec[k]<-Amat[i,j]
    }
  }
}
```

```

    }
  }
  svec
}

svec2mat <- function(svec){
  n2<-length(svec)
  n <- (-1+sqrt(1+8*n2))/2
  Amat <- matrix(0, nrow=n, ncol=n)
  k <- 0
  for (i in 1:n){
    for (j in 1:i){
      k<-k+1
      Amat[j,i]<-Amat[i,j]<-svec[k]
    }
  }
  Amat
}

n <- 4
AA <- FrankMat(n)
vv <- smat2vec(AA)
vv

```

```
## [1] 1 1 2 1 2 3 1 2 3 4
```

```
vinv<-A9(vv, n)
vinv
```

```
## [1] 2 -1 2 0 -1 2 0 0 -1 1
```

```
print(vinv)
```

```
## [1] 2 -1 2 0 -1 2 0 0 -1 1
```

```
Ainv<-svec2mat(vinv)
print(Ainv)
```

```
##      [,1] [,2] [,3] [,4]
## [1,]    2  -1    0    0
## [2,]   -1    2  -1    0
## [3,]    0  -1    2   -1
## [4,]    0    0  -1    1
```

```
print(Ainv %*% AA)
```

```
##      [,1] [,2] [,3] [,4]
## [1,]    1    0    0    0
## [2,]    0    1    0    0
## [3,]    0    0    1    0
## [4,]    0    0    0    1
```

Others

Algorithm 10 – Inverse iteration via Gaussian elimination

The purpose of this algorithm is to find a single eigensolution of a matrix A via inverse iteration. That is, we want solutions (e, x) of

$$Ax = ex$$

The programs do not require a symmetric matrix, which leaves open the possibility that a solution may not exist in the unsymmetric case.

Fortran

The Algorithm 10 code:

```
C TEST ALGORITHM 10 USING HILBERT SEGMENT
C J.C. NASH JULY 1978, APRIL 1989
  INTEGER N,N2,I,J,JN,NOUT
  REAL W(10,20),X(10),Y(10),SHIFT,EPS,S
C PRINTER CHANNEL
  NOUT=6
C MACHINE PRECISION NOTE -- IBM SHORT PRECISION
  EPS=16.0**(-5)
C MAIN LOOP
  DO 100 N=5,10,5
C CREATE HILBERT SEGMENT & UNIT MATRIX
  N2=2*N
  DO 20 I=1,N
    DO 10 J=1,N
      JN=J+N
      W(I,J)=1.0/(I+J-1)
      W(I,JN)=0.0
10    CONTINUE
      JN=N+I
      W(I,JN)=1.0
20    CONTINUE
      WRITE(NOUT,950)N
950    FORMAT(' ORDER=',I4)
      SHIFT=0.0
      WRITE(NOUT, 960)SHIFT
960    FORMAT(' USING SHIFT OF ',F12.6)
C SET GUESS TO VECTOR
  DO 30 I=1,N
    X(I)=1.0
30  CONTINUE
C SHOULD INPUT SHIFT
  LIMIT=10*N
C SET OUTPUT CHANNEL TO 0 TO SUPPRESS OUTPUT (ELSE USE NOUT)
  CALL A10GII(W,10,N,N2,X,Y,SHIFT,EPS,LIMIT,EV,0)
  WRITE(NOUT,951)EV,LIMIT
951  FORMAT(' CONVERGED TO EV=',1PE16.8,' IN ',I4,' ITERATIONS')
  WRITE(NOUT,952)(I,X(I),I=1,N)
952  FORMAT(' X(',I3,')=',E16.8)
  DO 50 I=1,N
    S=EV*X(I)
    DO 40 J=1,N
```

```

        S=S-X(J)/(I+J-1)
40    CONTINUE
        WRITE(NOUT,953)I,S
953   FORMAT(' RESIDUAL(',I3,')=',E16.8)
50    CONTINUE
100   CONTINUE
        STOP
        END
        SUBROUTINE A10GII(W,NW,N,N2,X,Y,SHIFT,EPS,LIMIT,EV,IPR)
C  ALGORITHM 10
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C  INVERSE ITERATION VIA GAUSS ELIMINATION
C  SOLVES EIGENPROBLEM A*X=EV*B*X FOR EIGENSOLUTION (EX,X)
C  VECTOR NORMALISED SO LARGEST ELEMENT IS 1.0
C  W=WORKING ARRAY HAVING INITIALLY A IN COLUMNS 1 TO N
C                                     B IN COLUMNS N+1 TO 2*N=N2
C  NW=FIRST DIMENSION OF W
C  N=ORDER OF PROBLEM
C  N2=2*N = NO. OF COLUMNS IN W
C  X = INITIAL GUESS FOR EIGENVECTOR - SHOULD NOT BE NULL
C  Y = WORKING VECTOR
C  X & Y OF LENGTH N AT LEAST
C  SHIFT = SHIFT TO TRANSFORM PROBLEM TO ONE WITH EV CLOSEST TO SHIFT
C  WITH EV CLOSEST TO SHIFT
C  EPS=MACHINE PRECISION--SMALLEST NUMBER S.T. 1.0+EPS.GT.1.0
C  LIMIT=UPPER BOUND TO NUMBER OF ITERATIONS
C  = ON OUTPUT THE NUMBER OF ITERATIONS USED
C  EV=EIGENVALUE CALCULATED
C  IPR=PRINT CHANNEL. IPR=0 SUPPRESSES PRINTING.
C  STEP 0
        INTEGER N,N2,NW,LIMIT,COUNT,I,J,JN,K,N1,I1
        REAL W(NW,N2),X(N),Y(N),EPS,SHIFT,EV,S,T,P
C  SAFETY CHECK
        IF(N2.NE.2*N)STOP
C  STEP 1
        T=0.0
        DO 10 I=1,N
            Y(I)=0.0
            S=0.0
            DO 5 J=1,N
                JN=J+N
                W(I,J)=W(I,J)-SHIFT*W(I,JN)
                S=S+ABS(W(I,J))
5        CONTINUE
            IF(T.LT.S)T=S
10    CONTINUE
        T=T*EPS
C  STEP 2
        N1=N-1
        DO 100 I=1,N1
C  STEP 3
            S=ABS(W(I,I))
            K=I

```

```

        I1=I+1
        DO 20 J=I1,N
            IF(ABS(W(J,I)).LE.S)GOTO 20
            S=ABS(W(J,I))
            K=J
20      CONTINUE
        IF(S.GT.0.0)GOTO 30
C   STEP 4
        W(I,I)=T
        GOTO 100
C   STEP 5
30      IF(K.EQ.I)GOTO 50
C   STEP 6
        DO 40 J=I,N2
            S=W(I,J)
            W(I,J)=W(K,J)
            W(K,J)=S
40      CONTINUE
C   STEP 7
50      DO 80 J=I1,N
            S=W(J,I)/W(I,I)
            DO 70 K=I,N2
                W(J,K)=W(J,K)-S*W(I,K)
70          CONTINUE
80      CONTINUE
C   STEP 8
100     CONTINUE
C   STEP 9
        IF(ABS(W(N,N)).EQ.0.0)W(N,N)=T
C   STEP 10
        COUNT=0
C   STEP 11
110     COUNT=COUNT+1
        M=N
        S=X(N)
        X(N)=Y(N)
        Y(N)=S/W(N,N)
        P=ABS(Y(N))
C   STEP 12
        DO 130 JN=1,N1
            I=N-JN
            S=X(I)
            X(I)=Y(I)
            I1=I+1
            DO 120 J=I1,N
                S=S-W(I,J)*Y(J)
120         CONTINUE
            Y(I)=S/W(I,I)
            IF(ABS(Y(I)).LE.P)GOTO 130
            P=ABS(Y(I))
            M=I
130     CONTINUE
C   STEP 13

```

```

      EV=SHIFT+X(M)/Y(M)
C  STEP 14
      P=Y(M)
      M=0
      DO 140 I=1,N
        Y(I)=Y(I)/P
        IF(FLOAT(N)+Y(I).EQ.FLOAT(N)+X(I))M=M+1
140  CONTINUE
      IF(IPR.GT.0)WRITE(IPR,960)COUNT,EV,M
960  FORMAT(14H ITERATION NO.,I4,14H   APPROX. EV=,1PE16.8,5X,I4,
        *27H VECTOR ELEMENTS TEST EQUAL)
C  STEP 15
      IF(M.EQ.N)GOTO 200
      IF(COUNT.GT.LIMIT)GOTO 200
C  STEP 16
      DO 160 I=1,N
        S=0.0
        DO 150 J=1,N
          JN=J+N
          S=S+W(I,JN)*Y(J)
150  CONTINUE
        X(I)=S
160  CONTINUE
C  STEP 17
      GOTO 110
200  LIMIT=COUNT
      RETURN
      END

```

Example output

We illustrate by finding a single eigensolution of the Hilbert segments of order 5 and 10. ?? Do we want to swap in the Frank matrix (the computations are generally easier)?

```

## #!/bin/bash
gfortran ../fortran/a10.f
mv ./a.out ../fortran/a10.run
../fortran/a10.run

```

```

## ORDER= 5
## USING SHIFT OF 0.000000
## CONVERGED TO EV= 3.29019417E-06 IN 5 ITERATIONS
## X( 1)= -0.80475118E-02
## X( 2)= 0.15210588E+00
## X( 3)= -0.65976608E+00
## X( 4)= 0.10000000E+01
## X( 5)= -0.49041715E+00
## RESIDUAL( 1)= -0.74505806E-08
## RESIDUAL( 2)= 0.00000000E+00
## RESIDUAL( 3)= -0.74505806E-08
## RESIDUAL( 4)= -0.37252903E-08
## RESIDUAL( 5)= -0.37252903E-08
## ORDER= 10
## USING SHIFT OF 0.000000
## CONVERGED TO EV= 1.26338462E-09 IN 101 ITERATIONS

```

```

## X( 1)= 0.50510102E-05
## X( 2)= -0.61139709E-03
## X( 3)= 0.65672603E-02
## X( 4)= -0.65278080E-02
## X( 5)= -0.94817474E-01
## X( 6)= 0.25418818E+00
## X( 7)= 0.62985711E-01
## X( 8)= -0.86295480E+00
## X( 9)= 0.10000000E+01
## X( 10)= -0.35897413E+00
## RESIDUAL( 1)= 0.00000000E+00
## RESIDUAL( 2)= 0.00000000E+00
## RESIDUAL( 3)= -0.18626451E-08
## RESIDUAL( 4)= -0.11175871E-07
## RESIDUAL( 5)= -0.37252903E-08
## RESIDUAL( 6)= 0.18626451E-08
## RESIDUAL( 7)= -0.18626451E-08
## RESIDUAL( 8)= -0.18626451E-08
## RESIDUAL( 9)= -0.37252903E-08
## RESIDUAL( 10)= 0.37252903E-08

```

BASIC

Listing

```

5 DIM A(10, 20),X(10),Y(10)
10 PRINT "GII JULY 25 77 ALG 10"
20 PRINT "GAUSS ELIMINATION FOR INVERSE ITERATION"
30 PRINT "ORDER=",
40 READ N
50 PRINT N
55 IF N <= 0 THEN QUIT : REM BWBASIC VARIANT
60 GOSUB 1500: REM BUILD OR INPUT MATRIX
70 GOSUB 2000: REM PUT METRIC IN RIGHT HALF OF A
75 GOSUB 1000: REM INITIAL GUESS TO VECTOR
80 LET K9=0 : REM SHIFT OF 0 FOR THIS EXAMPLE
90 PRINT "SHIFT=",K9
95 LET E9=K9
100 REM PRINT
105 LET T2=N: REM FACTOR FOR CONVERGENCE TEST
110 LET T1=0: REM STEP 1
120 FOR I=1 TO N
130 LET Q=0
140 FOR J=1 TO N
150 LET A(I,J)=A(I,J)-K9*A(I,J+N)
160 LET S=S+ABS(A(I,J))
170 NEXT J
180 IF T1>=S THEN GOTO 200
190 LET T1=S
200 NEXT I
205 LET T1=T1*1.0E-7: REM NS 8 DIGIT BASIC
210 FOR I=1 TO N-1: REM STEP 2
218 LET S=ABS(A(I,I)): REM STEP 3
226 LET K=I

```

```

234 FOR J=I+1 TO N
242 IF ABS(A(J,I))<=S THEN GOTO 266
250 LET S=ABS(A(J,I))
258 LET K=J
266 NEXT J
274 IF S>0 THEN GOTO 298: REM STEP 4
282 LET A(I,I)=T1
290 GOTO 394
298 IF K=I THEN GOTO 346: REM STEP 5
306 FOR J=I TO 2*N: REM STEP 6
314 LET S=A(I,J)
322 LET A(I,J)=A(K,J)
330 LET A(K,J)=S
338 NEXT J
346 FOR J=I+1 TO N: REM STEP 7
354 LET S=A(J,I)/A(I,I)
362 FOR K=I TO 2*N
370 LET A(J,K)=A(J,K)-S*A(I,K)
378 NEXT K
386 NEXT J
394 NEXT I: REM STEP 8
402 IF ABS(A(N,N))>0 THEN GOTO 420: REM STEP 9
410 LET A(N,N)=T1
420 LET I9=0: REM STEP 10
430 LET I9=I9+1: REM STEP 11
440 LET M=N
445 LET S=X(N)
450 LET X(N)=Y(N)
455 LET Y(N)=S/A(N,N)
460 LET P=ABS(Y(N))
470 FOR I=(N-1) TO 1 STEP -1: REM STEP 12
480 LET S=X(I)
485 LET X(I)=Y(I)
490 FOR J=I+1 TO N
500 LET S=S-A(I,J)*Y(J)
510 NEXT J
520 LET Y(I)=S/A(I,I)
530 IF ABS(Y(I))<=P THEN GOTO 560
540 LET M=I
550 LET P=ABS(Y(I))
560 NEXT I
570 LET E8=K9+X(M)/Y(M): REM STEP 13
580 REM PRINT "APPROX EV=",E8
600 LET P=Y(M): REM STEP 14
610 LET M=0
620 FOR I=1 TO N
630 LET Y(I)=Y(I)/P
635 IF T2+Y(I)<>T2+X(I) THEN GOTO 640
636 LET M=M+1
640 NEXT I
644 IF M=N THEN GOTO 730: REM STEP 15 -- CONVERGENCE TEST
645 IF I9>100 THEN GOTO 730: REM LIMIT SET AT 100
650 FOR I=1 TO N: REM STEP 16

```



```

660 LET S=0
670 FOR J=1 TO N
680 LET S=S+A(I,J+N)*Y(J)
690 NEXT J
700 LET X(I)=S
710 NEXT I
720 GOTO 430: REM STEP 17
725 REM STEP 18 -- END AND RESIDUALS
730 PRINT "CONVERGED TO EV=",E8," IN ",I9," ITNS"
735 PRINT M," EQUAL CPNTS IN VECTOR BETWEEN ITERATIONS"
740 GOSUB 1500: REM GET MATRIX AGAIN
750 GOSUB 2000: REM GET METRIC AGAIN
755 LET S=0: REM COMPUTE VECTOR INNER PRODUCT
760 FOR I=1 TO N
770 FOR J=1 TO N
780 LET S=S+Y(I)*A(I,J+N)*Y(J)
790 NEXT J
800 NEXT I
810 LET S=1/SQR(S)
815 PRINT "VECTOR"
820 FOR I=1 TO N
830 LET Y(I)=Y(I)*S: REM VECTOR NORMALIZATION
840 PRINT Y(I);
845 IF I=5*INT(I/5) THEN PRINT
850 NEXT I
855 PRINT
860 PRINT "RESIDUALS"
870 FOR I=1 TO N
880 LET S=0
890 FOR J=1 TO N: REM MATRIX * VECTOR - VALUE * METRIC * VECTOR
900 LET S=S+(A(I,J)-E8*A(I,J+N))*Y(J)
910 NEXT J
920 PRINT S;
925 IF 5*INT(I/5)=I THEN PRINT
930 NEXT I
940 PRINT
950 GOTO 40 : REM NEXT TRY
960 DATA 5, 10, -1
1000 REM INITIAL X
1010 FOR I=1 TO N
1020 LET X(I)=1: REM MAY BE A POOR CHOICE
1030 NEXT I
1040 RETURN
1500 REM A IN FOR FRANK MATRIX
1505 PRINT "FRANK MATRIX"
1510 FOR I=1 TO N
1520 FOR J=1 TO I
1530 A(I,J)=J
1540 A(J,I)=J
1550 NEXT J
1560 NEXT I
1570 RETURN
2000 REM UNIT B IN RIGHT HALF OF MATRIX

```

```

2010 FOR I=1 TO N
2020 FOR J=1 TO N
2030 A(I,J+N)=0
2040 NEXT J
2050 A(I,I+N)=1
2060 NEXT I
2070 RETURN

```

Example output

In this case we use the Frank matrix for our test.

```

bwbasic ../BASIC/a10.bas >../BASIC/a10.out
# echo "done"

```

Bywater BASIC Interpreter/Shell, version 2.20 patch level 2

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```

GII JULY 25 77 ALG 10
GAUSS ELIMINATION FOR INVERSE ITERATION
ORDER=
 5
FRANK MATRIX
SHIFT= 0
CONVERGED TO EV= 0.2715541 IN 101 ITNS
 1 EQUAL CPNTS IN VECTOR BETWEEN ITERATIONS
FRANK MATRIX
VECTOR
 0.3260187 -0.5485287 0.5968848 -0.4557341 0.1698911

RESIDUALS
-0 0 -0 -0 0

10
FRANK MATRIX
SHIFT= 0
CONVERGED TO EV= 0.2556738 IN 101 ITNS
 1 EQUAL CPNTS IN VECTOR BETWEEN ITERATIONS
FRANK MATRIX
VECTOR
 0.1281224 -0.2449948 0.3403202 -0.405639 0.4350771
-0.4258922 0.3787616 -0.2977698 0.1900823 -0.0653188

RESIDUALS
-0.0000087 0.0000141 -0.0000143 0.000009 -0
-0.0000097 0.0000166 -0.0000183 0.0000141 -0.0000053

-1

```

Pascal

Listing

```
program dr10(input,output);
{dr10.pas == driver to use Gauss elimination for inverse iteration
calculation of matrix eigensolutions

      Copyright 1988 J.C.Nash
}
{constype.def ==
  This file contains various definitions and type statements which are
  used throughout the collection of "Compact Numerical Methods". In many
  cases not all definitions are needed, and users with very tight memory
  constraints may wish to remove some of the lines of this file when
  compiling certain programs.

  Modified for Turbo Pascal 5.0

      Copyright 1988, 1990 J.C.Nash
}

const
  big = 1.0E+35;    {a very large number}
  Maxconst = 25;    {Maximum number of constants in data record}
  Maxobs = 100;     {Maximum number of observations in data record}
  Maxparm = 25;     {Maximum number of parameters to adjust}
  Maxvars = 10;     {Maximum number of variables in data record}
  acctol = 0.0001;  {acceptable point tolerance for minimisation codes}
  maxm = 20;        {Maximum number or rows in a matrix}
  maxn = 20;        {Maximum number of columns in a matrix}
  maxmn = 40;       {maxn+maxm, the number of rows in a working array}
  maxsym = 210;     {maximum number of elements of a symmetric matrix
                    which need to be stored = maxm * (maxm + 1)/2 }
  reltest = 10.0;   {a relative size used to check equality of numbers.
                    Numbers x and y are considered equal if the
                    floating-point representation of reltest*x equals
                    that of reltest*y.}
  stepredn = 0.2;   {factor to reduce stepsize in line search}
  yearwrit = 1990;  {year in which file was written}

type
  str2 = string[2];
  rmatrix = array[1..maxm, 1..maxn] of real; {a real matrix}
  wmatrix = array[1..maxmn, 1..maxn] of real; {a working array, formed
                    as one real matrix stacked on another}
  smatvec = array[1..maxsym] of real; {a vector to store a symmetric matrix
                    as the row-wise expansion of its lower triangle}
  rvector = array[1..maxm] of real; {a real vector. We will use vectors
                    of m elements always. While this is NOT space efficient,
                    it simplifies program codes.}
  cgmethodtype= (Fletcher_Reeves,Polak_Ribiere,Beale_Sorenson);
  {three possible forms of the conjugate gradients updating formulae}
  probdata = record
```

```

    m      : integer; {number of observations}
    nvar   : integer; {number of variables}
    nconst : integer; {number of constants}
    vconst : array[1..Maxconst] of real;
    Ydata  : array[1..Maxobs, 1..Maxvars] of real;
    nlls   : boolean; {true if problem is nonlinear least squares}
end;

{
  NOTE: Pascal does not let us define the work-space for the function
  within the user-defined code. This is a weakness of Pascal for this
  type of work.
}

var {global definitions}
    banner      : string[80]; {program name and description}

function calceps:real;
{calceps.pas ==
  This function returns the machine EPSILON or floating point tolerance,
  the smallest positive real number such that 1.0 + EPSILON > 1.0.
  EPSILON is needed to set various tolerances for different algorithms.
  While it could be entered as a constant, I prefer to calculate it, since
  users tend to move software between machines without paying attention to
  the computing environment. Note that more complete routines exist.
}
var
    e,e0: real;
    i: integer;
begin {calculate machine epsilon}
    e0 := 1; i:=0;
    repeat
        e0 := e0/2; e := 1+e0; i := i+1;
    until (e=1.0) or (i=50); {note safety check}
    e0 := e0*2;
{ Writeln('Machine EPSILON =',e0);}
    calceps:=e0;
end; {calceps}

function genevres(n: integer; {order of matrices}
    A, B: rmatrix;
    evalue : real; {eigenvalue}
    X : rvector; {presumed eigenvector}
    print: boolean) {true for printing}
    : real; {returns sum of squared residuals}

{genevres.pas

  -- to compute residuals of generalized (symmetric) matrix
  eigenvalue problem

    A x = evalue B x
}

```

```

var
  t, ss : real;
  i,j : integer;

begin
  if print then
    begin
      writeln('Generalized matrix eigensolution residuals');
    end;
  ss:=0.0; {to accumulate the sum of squared residuals}
  for i:=1 to n do
    begin
      t:=0.0;
      for j:=1 to n do
        t:=t+(A[i,j]-evalue*B[i,j])*X[j];
        if print then
          begin
            write(t:10,' ');
            if (7 * (i div 7) = i) and (i<n) then writeln;
          end; {if print}
        ss:=ss+t*t;
      end;
    end;
  if print then
    begin
      writeln;
      writeln('Sum of squared residuals =',ss);
    end; {if print}
  genevres:=ss; {return sum of squared residuals}
end; {genevres.pas == residuals for generalized eigenproblem}

function rayquo(n :integer;
  A,B : rmatrix;
  Y : rvector): real;
{rayquo.pas
  == compute Rayleigh quotient. If the denominator of
  the quotient is zero, set the quotient to a large
  negative number (-big)
}
var
  s,t : real;
  i,j : integer;

begin
  s:=0.0; t:=0.0;
  for i:=1 to n do
    begin
      for j:=1 to n do
        begin
          s:=s+Y[i]*A[i,j]*Y[j];
          t:=t+Y[i]*B[i,j]*Y[j];
        end; {loop on j}
      end; {loop on i}
    if t>0.0 then rayquo:=s/t else rayquo:=-big;
    {note the safety value for the result}
  end;

```

```

end; {rayquo.pas == compute Rayleigh quotient}

Procedure Frank2(var m, n: integer; var A: rmatrix);
var
  i,j: integer;
begin
  for i:=1 to m do
    begin
      for j:=1 to n do
        begin
          if (i <= j) then
            A[i,j]:=i
          else
            A[i,j]:=j;
          end;
        end;
      end;
    end;
  end;

Procedure gelim( n : integer;
                 p : integer;
                 var A : rmatrix;
                 tol : real);

var
  det, s : real;
  h,i,j,k: integer;

begin
  det := 1.0;
  writeln('alg05.pas -- Gauss elimination with partial pivoting');
  for j := 1 to (n-1) do
    begin
      s := abs(A[j,j]); k := j;
      for h := (j+1) to n do
        begin
          if abs(A[h,j])>s then
            begin
              s := abs(A[h,j]); k := h;
            end;
          end;
      if k<>j then
        begin
          writeln('Interchanging rows ',k,' and ',j);
          for i := j to (n+p) do
            begin
              s := A[k,i]; A[k,i] := A[j,i]; A[j,i] := s;
            end;
          det := -det;
        end;
      det := det*A[j,j];
      if abs(A[j,j])<tol then
        begin

```

```

        writeln('Matrix computationally singular -- pivot < ',tol);
        halt;
    end;
    for k := (j+1) to n do
    begin
        A[k,j] := A[k,j]/A[j,j];
        for i := (j+1) to (n+p) do
            A[k,i] := A[k,i]-A[k,j]*A[j,i];
        end;
        det := det*A[n,n];
        if abs(A[n,n])<tol then
        begin
            writeln('Matrix computationally singular -- pivot < ',tol);
            halt;
        end;
    end;
    writeln('Gauss elimination complete -- determinant = ',det);
end;

procedure gii(nRow : integer;
              var A : rmatrix;
              var Y : rvector;
              var shift : real;
              var itcount: integer);

var
    i, itlimit, j, m, msame, nRHS :integer;
    ev, s, t, tol : real;
    X : rvector;

begin
    itlimit:=itcount;
    nRHS:=nRow;
    tol:=Calceps;
    s:=0.0;
    for i:=1 to nRow do
    begin
        X[i]:=Y[i];
        Y[i]:=0.0;
        for j:=1 to nRow do
        begin
            A[i,j]:=A[i,j]-shift*A[i,j+nRow];
            s:=s+abs(A[i,j]);
        end;
    end;
    tol:=tol*s;
    gelim(nRow, nRHS, A, tol);
    itcount:=0;
    msame :=0;
    while (msame<nRow) and (itcount<itlimit) do
    begin
        itcount:=itcount+1;
        m:=nRow; s:=X[nRow];
        X[nRow]:=Y[nRow];
    end;
end;

```

```

    if abs(A[nRow,nRow])<tol then Y[nRow]:=s/tol
                                   else Y[nRow]:=s/A[nRow,nRow];
t:=abs(Y[nRow]);
for i:=(nRow-1) downto 1 do
begin
    s:=X[i]; X[i]:=Y[i];
    for j:=(i+1) to nRow do
    begin
        s:=s-A[i,j]*Y[j];
    end;
    if abs(A[i,i])<tol then Y[i]:=s/tol else Y[i]:=s/A[i,i];
    if abs(Y[i])>t then
    begin
        m:=i; t:=abs(Y[i]);
    end;
end;
ev:=shift+X[m]/Y[m];
(*   writeln('Iteration ',itcount,' approx. ev=',ev);*)

t:=Y[m]; msame:=0;
for i:=1 to nRow do
begin
    Y[i]:=Y[i]/t;
    if reltest+Y[i] = reltest+X[i] then msame:=msame+1;

end;

if msame<nRow then
begin
    for i:=1 to nRow do
    begin
        s:=0.0;
        for j:=1 to nRow do s:=s+A[i,j+nRow]*Y[j];
        X[i]:=s;
    end;
end;
end;
if itcount>=itlimit then itcount:=-itcount;
shift:=ev;
end;

var
    A, Acopy, B, Bcopy : rmatrix;
    Y : rvector;
    i, itcount, j, n, nRow, nCol : integer;
    rq, ss, Shift : real;
    vectorOK : boolean;

begin
    banner:='dr10.pas -- inverse iteration via Gauss elimination';
    repeat
        write('order of problem (n) = '); readln(n);
        writeln(n);

```



```

if (n > 0) then
begin {main loop over examples}
  nRow:=n; nCol:=2*n; {store matrices in an array n by 2n}
  writeln('Provide the A matrix');
  Frank2(nRow, nCol, Acopy);
  writeln('A matrix');
  for i:=1 to n do
  begin
    for j:=1 to n do
    begin
      write(Acopy[i,j]:10:5,' ');
      if (7 * (j div 7) = j) and (j<n) then writeln;
    end;
    writeln;
  end;
  writeln('B matrix set to unit matrix');
  for i:=1 to n do
  begin
    for j:=1 to n do B[i,j]:=0.0;
    Bcopy[i,i]:=1.0;
  end;
  writeln('B matrix');
  for i:=1 to n do
  begin
    for j:=1 to n do
    begin
      write(Bcopy[i,j]:10:5,' ');
      if (7 * (j div 7) = j) and (j<n) then writeln;
    end;
    writeln;
  end;
  shift:=0.0; {rem initial and safety value for the eigenvalue shift}
  vectorOK:=true; {approximate eigenvector will be all 1s for example}
  for i:=1 to n do Y[i]:=1.0; {Set starting vector}
  repeat
  if (not vectorOK) then
  begin
    writeln('Need a starting vector for inverse iteration');
    halt;
  end;
  vectorOK:=true; {set flag to indicate a vector is now in place}
(*
  writeln('Enter a shift for eigenvalues ([cr] = ',shift,') ');
  write(' A value > 1E+30 halts execution. Entry = ');
*)
  write('shift=?');
  readln(shift);
  writeln(shift);
  if (not (shift > 1e30)) then
  begin
    for i:=1 to n do {copy matrices into working matrices}
    begin
      for j:=1 to n do

```

```

begin
  A[i,j]:=Acopy[i,j]; B[i,j]:=Bcopy[i,j];
  A[i,j+n]:=B[i,j]; {to provide work matrix for ALG10}
end; {loop on j}
end; {loop on i}
itcount:=100; {rem fairly liberal bound}
gii(n, A , Y, shift, itcount);
writeln;
if itcount > 0 then
begin
  writeln(
    'Converged to eigenvalue =',shift,' in ',itcount,' iterations');
end
else
begin
  writeln('Not converged. Approximate eigenvalue=',shift,
    ' after ',-itcount,' iterations');
end; {else not converged}
writeln('Eigenvector');
for i:=1 to n do
begin
  write(Y[i]:10:5,' ');
  if (7* (i div 7) = i) and (i<n) then writeln;
end; {loop on i}
writeln;
ss:=genevres(n, Acopy, Bcopy, shift, Y, false);
rq:=rayquo(n, Acopy, Bcopy, Y);
writeln('Rayleigh quotient = ',rq,' sumsquared err=',ss:12:9);
end; {if shift <=1e30}
until (shift>1e30); {end of loop over possible shifts}
end; {main loop over n block}
until (n <= 0);
end. {dr10.pas}

```

Example output

```

fpc ../Pascal2021/dr10.pas
# copy to run file
mv ../Pascal2021/dr10 ../Pascal2021/dr10.run
../Pascal2021/dr10.run <../Pascal2021/dr10p.in >../Pascal2021/dr10p.out

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr10.pas
## Linking ../Pascal2021/dr10
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 402 lines compiled, 0.1 sec

order of problem (n) = 5
Provide the A matrix
A matrix
  1.00000  1.00000  1.00000  1.00000  1.00000
  1.00000  2.00000  2.00000  2.00000  2.00000

```

```

1.00000  2.00000  3.00000  3.00000  3.00000
1.00000  2.00000  3.00000  4.00000  4.00000
1.00000  2.00000  3.00000  4.00000  5.00000
B matrix set to unit matrix
B matrix
1.00000  0.00000  0.00000  0.00000  0.00000
0.00000  1.00000  0.00000  0.00000  0.00000
0.00000  0.00000  1.00000  0.00000  0.00000
0.00000  0.00000  0.00000  1.00000  0.00000
0.00000  0.00000  0.00000  0.00000  1.00000
shift=? 0.0000000000000000E+000
alg05.pas -- Gauss elimination with partial pivoting
Gauss elimination complete -- determinant = 2.4000000000000000E+001

Not converged. Approximate eigenvalue= 2.7155412933904033E-001 after 100 iterations
Eigenvector
0.54620 -0.91899 1.00000 -0.76352 0.28463
Rayleigh quotient = 2.7155412933882112E-001 sumsquared err= 0.000000000
shift=? 1.0000000000000001E+032
order of problem (n) = 10
Provide the A matrix
A matrix
1.00000  1.00000  1.00000  1.00000  1.00000  1.00000  1.00000
1.00000  1.00000  1.00000
1.00000  2.00000  2.00000  2.00000  2.00000  2.00000  2.00000
2.00000  2.00000  2.00000
1.00000  2.00000  3.00000  3.00000  3.00000  3.00000  3.00000
3.00000  3.00000  3.00000
1.00000  2.00000  3.00000  4.00000  4.00000  4.00000  4.00000
4.00000  4.00000  4.00000
1.00000  2.00000  3.00000  4.00000  5.00000  5.00000  5.00000
5.00000  5.00000  5.00000
1.00000  2.00000  3.00000  4.00000  5.00000  6.00000  6.00000
6.00000  6.00000  6.00000
1.00000  2.00000  3.00000  4.00000  5.00000  6.00000  7.00000
7.00000  7.00000  7.00000
1.00000  2.00000  3.00000  4.00000  5.00000  6.00000  7.00000
8.00000  8.00000  8.00000
1.00000  2.00000  3.00000  4.00000  5.00000  6.00000  7.00000
8.00000  9.00000  9.00000
1.00000  2.00000  3.00000  4.00000  5.00000  6.00000  7.00000
8.00000  9.00000  10.00000
B matrix set to unit matrix
B matrix
1.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
0.00000  0.00000  0.00000
0.00000  1.00000  0.00000  0.00000  0.00000  0.00000  0.00000
0.00000  0.00000  0.00000
0.00000  0.00000  1.00000  0.00000  0.00000  0.00000  0.00000
0.00000  0.00000  0.00000
0.00000  0.00000  0.00000  1.00000  0.00000  0.00000  0.00000
0.00000  0.00000  0.00000
0.00000  0.00000  0.00000  0.00000  1.00000  0.00000  0.00000

```

```

0.00000  0.00000  0.00000
0.00000  0.00000  0.00000  0.00000  0.00000  1.00000  0.00000
0.00000  0.00000  0.00000
0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  1.00000
0.00000  0.00000  0.00000
0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
1.00000  0.00000  0.00000
0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
0.00000  1.00000  0.00000
0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
0.00000  0.00000  1.00000
shift=? 0.0000000000000000E+000
alg05.pas -- Gauss elimination with partial pivoting
Gauss elimination complete -- determinant = 3.6288000000000000E+005

Not converged. Approximate eigenvalue= 2.5567344134720177E-001 after 100 iterations
Eigenvector
  0.29440  -0.56298  0.78208  -0.93226  1.00000  -0.97898  0.87071
 -0.68457  0.43702  -0.15018
Rayleigh quotient = 2.5567965533013154E-001  sumsqared err= 0.000000009
shift=? 1.0000000000000001E+032
order of problem (n) = 0

```

Algorithms 11 and 12 – standardization and residuals for a complex eigensolution

These algorithms are probably among the least used of those included in Nashlib. Their intent was to allow proposed eigensolutions of complex matrices to be standardized and tested. This seemed a potentially important task in the 1970s. ?? include COMEIG (ref to Eberlein's work, others??)

The purpose of standardization is to facilitate comparisons between eigenvectors that are supposedly equivalent. Any (preferably) unit-length multiple of an eigenvector is also an eigenvector, so it is difficult to compare two proposed solutions for the same eigenvalue. Therefore we choose a multiplier so that the largest magnitude component of the eigenvector is set to $1 + 0i$ where

$$i = \sqrt{-1}$$

Fortran

The Algorithm 11 and 12 code:

```
C&&& A1112
C  TEST ALGORITHMS 11 & 12
C  J.C. NASH    JULY 1978, APRIL 1989
      INTEGER N,NS,NIN,NOUT
      REAL A(10,10),Z(10,10),X(10),Y(10),U(10),V(10),E,F,VNORM
      NA=10
      NIN=5
      NOUT=6
10  READ(NIN,905)N
905  FORMAT(I5)
      WRITE(NOUT,965)N
965  FORMAT(' ORDER=',I4)
      IF(N.LE.0)STOP
C  READ MATRICES
      DO 20 I=1,N
          READ(NIN,906) (A(I,J),J=1,N)
906  FORMAT(6F10.5)
20  CONTINUE
      WRITE(NOUT,966)
966  FORMAT(' MATRIX A')
      CALL OUT(A,NA,N,N,NOUT)
      DO 30 I=1,N
          READ(NIN,906) (Z(I,J),J=1,N)
30  CONTINUE
      WRITE(NOUT,967)
967  FORMAT(' MATRIX Z')
      CALL OUT(Z,NA,N,N,NOUT)
40  READ(NIN,907)NS,E,F
907  FORMAT(I5,5X,2F10.5)
      WRITE(NOUT,968)NS,E,F
968  FORMAT(' SOLUTION',I4,' EV=',1PE16.8,' + SQRT(-1)*',E16.8)
      IF(NS.LE.0)GOTO 10
      READ(NIN,906) (X(J),J=1,N)
      WRITE(NOUT,969)
969  FORMAT(' REAL PART')
      WRITE(NOUT,970) (X(J),J=1,N)
970  FORMAT(1H ,6E16.8)
```

```

        READ(NIN,906) (Y(J),J=1,N)
        WRITE(NOUT,971)
971  FORMAT(' IMAGINARY PART')
        WRITE(NOUT,970) (Y(J),J=1,N)
        CALL A11VS(N,X,Y,VNORM)
        WRITE(NOUT,972) VNORM
972  FORMAT(' STANDARDIZED VECTOR - NORM=',1PE16.8)
        WRITE(NOUT,969)
        WRITE(NOUT,970) (X(J),J=1,N)
        WRITE(NOUT,971)
        WRITE(NOUT,970) (Y(J),J=1,N)
        WRITE(NOUT,973)
973  FORMAT(' RESIDUALS')
        CALL A12CVR(N,X,Y,A,10,Z,10,E,F,U,V)
        WRITE(NOUT,969)
        WRITE(NOUT,970) (U(J),J=1,N)
        WRITE(NOUT,971)
        WRITE(NOUT,970) (V(J),J=1,N)
        GOTO 40
    END
    SUBROUTINE A11VS(N,X,Y,VNORM)
C  ALGORITHM 11 - COMPLEX VECTOR STANDARDISATION
C  J.C. NASH JULY 1978, FEBRUARY 1980, APRIL 1989
C  STANDARDISES COMPLEX VECTOR (N ELEMENTS)  $X + \sqrt{-1} * Y$ 
C  TO  $1.0 + \sqrt{-1} * 0.0$ 
C  VNORM = NORM OF VECTOR (LARGEST ELEMENT)
C  STEP 0
        INTEGER N,I,K
        REAL X(N),Y(N),VNORM,G,B,E,S
C  STEP 1
        G=0.0
C  STEP 2
        DO 60 I=1,N
C  STEP 3
            B=X(I)**2+Y(I)**2
C  STEP 4
            IF(B.LE.G)GOTO 60
C  STEP 5
            K=I
            G=B
C  STEP 6
60  CONTINUE
C  SAVE NORM
        VNORM=G
C  SAFETY CHECK
        IF(G.EQ.0.0)RETURN
C  STEP 7
        E=X(K)/G
        S=-Y(K)/G
C  STEP 8
        DO 85 I=1,N
            G=X(I)*E-Y(I)*S
            Y(I)=Y(I)*E+X(I)*S

```

```

        X(I)=G
85  CONTINUE
C  END
    RETURN
    END
    SUBROUTINE A12CVR(N,X,Y,A,NA,Z,NZ,E,F,U,V)
C  ALGORITHM 12 RESIDUALS OF A COMPLEX EIGENSOLUTION
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C  N          = ORDER OF PROBLEM
C  U + I*V = ( A + I*Z - E - I*F)*(X + I*Y)  WHERE I=SQRT(-1)
C  NA,NZ = FIRST DIMENSIONS OF A & Z RESPECTIVELY
C  STEP 0
        INTEGER N,NA,NZ,J,K
        REAL A(NA,N),Z(NZ,N),X(N),Y(N),E,F,U(N),V(N),S,G
C  STEP 1
        DO 50 J=1,N
C  STEP 2
            S=-E*X(J)+F*Y(J)
            G=-F*X(J)-E*Y(J)
C  STEP 3
            DO 35 K=1,N
                S=S+A(J,K)*X(K)-Z(J,K)*Y(K)
                G=G+A(J,K)*Y(K)+Z(J,K)*X(K)
35      CONTINUE
C  STEP 4  NOTE SAVE IN U & V
            U(J)=S
            V(J)=G
C  STEP 5
50  CONTINUE
    RETURN
    END
    SUBROUTINE OUT(A,NA,N,NP,NOUT)
C  J.C. NASH    JULY 1978, APRIL 1989
    INTEGER NA,N,NOUT,I,J
    REAL A(NA,N)
    DO 20 I=1,N
        WRITE(NOUT,951)I
951    FORMAT(' ROW',I3)
        WRITE(NOUT,952)(A(I,J),J=1,NP)
952    FORMAT(1H ,1P5E16.8)
20  CONTINUE
    RETURN
    END

```

Example output

We illustrate by finding a single eigensolution of the Hilbert segments of order 5 and 10. ?? Do we want to swap in the Frank matrix (the computations are generally easier)?

```

## #!/bin/bash
gfortran ../fortran/a1112.f
mv ./a.out ../fortran/a1112.run
../fortran/a1112.run <../fortran/a1112.in

```

```
## ORDER= 2
```

```

## MATRIX A
## ROW 1
## 1.00000000E+00 0.00000000E+00
## ROW 2
## 0.00000000E+00 1.00000000E+00
## MATRIX Z
## ROW 1
## 0.00000000E+00 -1.00000000E+00
## ROW 2
## 1.00000000E+00 0.00000000E+00
## SOLUTION 1 EV= 2.00000000E+00 + SQRT(-1)* 0.00000000E+00
## REAL PART
## 0.50000000E+00 0.00000000E+00
## IMAGINARY PART
## 0.00000000E+00 0.50000000E+00
## STANDARDIZED VECTOR - NORM= 2.50000000E-01
## REAL PART
## 0.10000000E+01 0.00000000E+00
## IMAGINARY PART
## 0.00000000E+00 0.10000000E+01
## RESIDUALS
## REAL PART
## 0.00000000E+00 0.00000000E+00
## IMAGINARY PART
## 0.00000000E+00 0.00000000E+00
## SOLUTION 2 EV= 0.00000000E+00 + SQRT(-1)* 0.00000000E+00
## REAL PART
## -0.10000000E+01 0.00000000E+00
## IMAGINARY PART
## 0.00000000E+00 0.10000000E+01
## STANDARDIZED VECTOR - NORM= 1.00000000E+00
## REAL PART
## 0.10000000E+01 0.00000000E+00
## IMAGINARY PART
## 0.00000000E+00 -0.10000000E+01
## RESIDUALS
## REAL PART
## 0.00000000E+00 0.00000000E+00
## IMAGINARY PART
## 0.00000000E+00 0.00000000E+00
## SOLUTION -1 EV= 0.00000000E+00 + SQRT(-1)* 0.00000000E+00
## ORDER= 2
## MATRIX A
## ROW 1
## 1.00000000E+00 1.00000000E+00
## ROW 2
## 1.00000000E+00 1.00000000E+00
## MATRIX Z
## ROW 1
## 0.00000000E+00 -1.00000000E+00
## ROW 2
## 1.00000000E+00 0.00000000E+00
## SOLUTION 1 EV= 2.41420007E+00 + SQRT(-1)* 0.00000000E+00
## REAL PART

```



```

##      0.14141999E+01  0.10000000E+01
## IMAGINARY PART
##      0.00000000E+00  0.10000000E+01
## STANDARDIZED VECTOR - NORM=  2.00000000E+00
## REAL PART
##      0.70709997E+00  0.10000000E+01
## IMAGINARY PART
##     -0.70709997E+00  0.00000000E+00
## RESIDUALS
## REAL PART
##      0.19133091E-04 -0.23841858E-06
## IMAGINARY PART
##     -0.19133091E-04  0.00000000E+00
## SOLUTION  2  EV= -5.85799992E-01 + SQRT(-1)*  0.00000000E+00
## REAL PART
##     -0.14141999E+01  0.10000000E+01
## IMAGINARY PART
##      0.00000000E+00  0.10000000E+01
## STANDARDIZED VECTOR - NORM=  2.00000000E+00
## REAL PART
##     -0.70709997E+00  0.10000000E+01
## IMAGINARY PART
##      0.70709997E+00  0.00000000E+00
## RESIDUALS
## REAL PART
##     -0.12131917E+00  0.17160004E+00
## IMAGINARY PART
##      0.12131917E+00  0.00000000E+00
## SOLUTION  0  EV=  0.00000000E+00 + SQRT(-1)*  0.00000000E+00
## ORDER=  3
## MATRIX A
## ROW  1
##      1.00000000E+00  2.00000000E+00  3.00000000E+00
## ROW  2
##      4.00000000E+00  5.00000000E+00  6.00000000E+00
## ROW  3
##      7.00000000E+00  8.00000000E+00  9.00000000E+00
## MATRIX Z
## ROW  1
##      9.00000000E+00  8.00000000E+00  7.00000000E+00
## ROW  2
##      6.00000000E+00  5.00000000E+00  4.00000000E+00
## ROW  3
##      3.00000000E+00  2.00000000E+00  1.00000000E+00
## SOLUTION  1  EV=  1.36844997E+01 + SQRT(-1)*  1.36844997E+01
## REAL PART
##      0.49906299E+00  0.56529301E+00  0.63152498E+00
## IMAGINARY PART
##      0.47247899E+00  0.10070200E+00 -0.27107400E+00
## STANDARDIZED VECTOR - NORM=  4.72304910E-01
## REAL PART
##      0.39612967E+00  0.69806379E+00  0.10000000E+01
## IMAGINARY PART
##      0.91818923E+00  0.45909339E+00  0.00000000E+00

```

```

## RESIDUALS
## REAL PART
## -0.69141388E-04 0.45776367E-04 0.16307831E-03
## IMAGINARY PART
## 0.25606155E-03 0.20432472E-03 0.89049339E-04
## SOLUTION 2 EV= 1.31529999E+00 + Sqrt(-1)* 1.31531000E+00
## REAL PART
## 0.74067497E+00 -0.24551900E-01 -0.78978002E+00
## IMAGINARY PART
## -0.27984101E+00 -0.11183600E+00 0.56165900E-01
## STANDARDIZED VECTOR - NORM= 6.26910388E-01
## REAL PART
## 0.10000000E+01 0.20914188E-01 -0.95817167E+00
## IMAGINARY PART
## 0.00000000E+00 -0.14309023E+00 -0.28618470E+00
## RESIDUALS
## REAL PART
## 0.27894974E-04 0.14424324E-04 -0.43809414E-05
## IMAGINARY PART
## 0.67234039E-04 0.22649765E-04 -0.16033649E-04
## SOLUTION 3 EV= 0.00000000E+00 + Sqrt(-1)* 0.00000000E+00
## REAL PART
## -0.40955499E+00 0.81911302E+00 -0.40955701E+00
## IMAGINARY PART
## -0.16320599E-01 0.32640599E-01 -0.16320400E-01
## STANDARDIZED VECTOR - NORM= 6.72011554E-01
## REAL PART
## -0.49999815E+00 0.10000000E+01 -0.50000060E+00
## IMAGINARY PART
## -0.43958426E-06 -0.37252903E-08 -0.96857548E-07
## RESIDUALS
## REAL PART
## 0.47311187E-05 0.68247318E-05 0.91567636E-05
## IMAGINARY PART
## 0.11682510E-04 0.64373016E-05 0.89406967E-06
## SOLUTION -1 EV= 0.00000000E+00 + Sqrt(-1)* 0.00000000E+00
## ORDER= 0

```

Pascal

?? Currently we do not seem to have an example driver for these two codes.

Listing – a11.pas

```

procedure stdceigv(n: integer;
                  var T, U: rmatrix);

var
  i, k, m : integer;
  b, e, g, s : real;

begin
  writeln('alg11.pas -- standardized eigensolutions');
  writeln(confile, 'alg11.pas -- standardized eigensolutions');

```

```

for i := 1 to n do
begin
  g := T[1,i]*T[1,i]+U[1,i]*U[1,i];

  k := 1;
  if n>1 then
  begin
    for m := 2 to n do
    begin
      b := T[m,i]*T[m,i]+U[m,i]*U[m,i];
      if b>g then
      begin
        k := m;
        g := b;
      end;
    end;
  end;
  e := T[k,i]/g;
  s := -U[k,i]/g;
  for k := 1 to n do
  begin
    g := T[k,i]*e-U[k,i]*s; U[k,i] := U[k,i]*e+T[k,i]*s; T[k,i] := g;
  end;
end;
end;

```

Listing – a12.pas

```

procedure comres( i, n: integer;
                  A, Z, T, U, Acopy, Zcopy : rmatrix);

var
  j, k: integer;
  g, s, ss : real;

begin
  writeln('alg12.pas -- complex eigensolution residuals');
  writeln(confile,'alg12.pas -- complex eigensolution residuals');
  ss := 0.0;
  for j := 1 to n do
  begin
    s := -A[i,i]*T[j,i]+Z[i,i]*U[j,i]; g := -Z[i,i]*T[j,i]-A[i,i]*U[j,i];

    for k := 1 to n do
    begin
      s := s+Acopy[j,k]*T[k,i]-Zcopy[j,k]*U[k,i];
      g := g+Acopy[j,k]*U[k,i]+Zcopy[j,k]*T[k,i];
    end;
    writeln('(' ,s ,',',g ,')'); writeln(confile,'(' ,s ,',',g ,')');
    ss := ss+s*s+g*g;
  end;
  writeln('Sum of squares = ',ss); writeln(confile,'Sum of squares = ',ss);
  writeln; writeln(confile);

```

```
end;
```

Algorithm 13

Fortran

Listing

```
C&&& A13
C TEST ALG. 13      JULY 1978
C J.C. NASH      JULY 1978, APRIL 1989
      REAL H,EPS
      INTEGER N,ND,I,NOUT,NIN
      REAL A(10,10),B(10,10),AT(10,10),Z(10),V(10,10),RMAX,VMAX
      EXTERNAL FRANKM,UNITM
      ND=10
C I/O CHANNELS
      NIN=5
      NOUT=6
      1 READ(NIN,900)N
      900 FORMAT(I4)
      WRITE(NOUT,901)N
      901 FORMAT(' ORDER N=',I4)
      IF(N.LE.0)STOP
      CALL FRANKM(N,N,V,ND)
      ISWP=30
C IBM SHORT PRECISION
      EPS=16.0**(-5)
C IBM VALUE FOR BIG NO.
C&&&      H=R1MACH(2)
      H = 1.0E+35
      CALL A13ESV(N,V,ND,EPS,H,ISWP,NOUT,Z)
      WRITE(NOUT,903)ISWP
      903 FORMAT(' CONVERGED IN ',I4,' SWEEPS')
      CALL EVT(N,V,ND,Z,FRANKM,UNITM,AT,ND,B,ND,NOUT,RMAX,VMAX)
      GOTO 1
      END
      SUBROUTINE A13ESV(N,A,NA,EPS,H,ISWP,IPR,Z)
C ALGORITHM 13 EIGENPROBLEM OF A REAL SYMMETRIC MATRIX VIA SVD
C J.C. NASH      JULY 1978, FEBRUARY 1980, APRIL 1989
C N      = ORDER OF PROBLEM
C A      = ARRAY CONTAINING MATRIX FOR WHICH EIGENVALUES ARE TO BE
C          COMPUTED. RETURNS EIGENVECTORS AS COLUMNS
C NA     = FIRST DIMENSION OF A
C EPS    = MACHINE PRECISION
C H      = A NUMBER LARGER THAN ANY POSSIBLE EIGENVALUE. CHANGED
C          DURING EXECUTION. DO NOT ENTER AS A CONSTANT
C ISWP   = LIMIT ON SWEEPS (INPUT). SWEEPS USED (OUTPUT).
C IPR    = PRINT CHANNEL. IPR.GT.0 FOR PRINTING.
C Z      = EIGENVALUES (OUTPUT)
C STEP 0
      INTEGER N,NA,ISWP,IPR,LISWP,I,J,COUNT,N1,J1
      REAL A(NA,N),EPS,H,V,Z(N),P,Q,R,S,C
      LISWP=ISWP
      ISWP=0
      N1=N-1
```

```

C  STEP 1
      DO 5 I=1,N
        V=A(I,I)
        DO 3 J=1,N
          IF(J.EQ.I)GOTO 3
          V=V-ABS(A(I,J))
3      CONTINUE
        IF(V.LT.H)H=V
5      CONTINUE
        IF(H.LE.EPS)GOTO 6
        H=0.0
        GOTO 30
6      H=H-SQRT(EPS)
C  STEP 2
      DO 15 I=1,N
        A(I,I)=A(I,I)-H
15     CONTINUE
C  STEP 3
30     COUNT=0
C  CHECK FOR ORDER 1 PROBLEMS AND SKIP WORK
      IF(N.EQ.1)GOTO 160
      ISWP=ISWP+1
      IF(ISWP.GT.LISWP)GOTO 160
C  STEP 4
      DO 140 J=1,N1
C  STEP 5
        J1=J+1
        DO 130 K=J1,N
C  STEP 6
          P=0.0
          Q=0.0
          R=0.0
          DO 65 I=1,N
            P=P+A(I,J)*A(I,K)
            Q=Q+A(I,J)**2
            R=R+A(I,K)**2
65         CONTINUE
C  STEP 7
          IF(1.0.LT.1.0+ABS(P/SQRT(Q*R)))GOTO 80
          IF(Q.LT.R)GOTO 80
          COUNT=COUNT+1
          GOTO 130
80         Q=Q-R
C  STEP 8
          V=SQRT(4.0*P*P+Q*Q)
          IF(V.EQ.0.0)GOTO 130
C  STEP 9
          IF(Q.LT.0.0)GOTO 110
C  STEP 10
          C=SQRT((V+Q)/(2.0*V))
          S=P/(V*C)
          GOTO 120
C  STEP 11

```

```

110      S=SQRT((V-Q)/(2.0*V))
        IF(P.LT.0.0)S=-S
        C=P/(V*S)
C  STEP 12
120      DO 125 I=1,N
        V=A(I,J)
        A(I,J)=V*C+A(I,K)*S
        A(I,K)=-V*S+A(I,K)*C
125      CONTINUE
C  STEP 13
130      CONTINUE
C  STEP 14
140      CONTINUE
C  STEP 15
        IF(IPR.GT.0)WRITE(IPR,970)ISWP,COUNT
970      FORMAT( 9H AT SWEEP,I4,2X,I4,18H ROTATIONS SKIPPED)
        IF(COUNT.LT.N*(N-1)/2)GOTO 30
C  STEP 16
160      DO 168 J=1,N
        S=0.0
        DO 162 I=1,N
        S=S+A(I,J)**2
162      CONTINUE
        S=SQRT(S)
        DO 164 I=1,N
        A(I,J)=A(I,J)/S
164      CONTINUE
        R=S+H
        Z(J)=R
168      CONTINUE
C  STEP 17
170      RETURN
        END
        SUBROUTINE UNITM(M,N,A,NA)
C  PUTS UNIT MATRIX M BY N IN A
C  J.C. NASH JULY 1978, APRIL 1989
        INTEGER M,N,NA,I,J
        REAL A(NA,N)
        DO 10 I=1,M
        DO 5 J=1,N
        A(I,J)=0.0
        IF(I.EQ.J)A(I,I)=1.0
5      CONTINUE
10     CONTINUE
        RETURN
        END
        SUBROUTINE EVT(N,V,NV,Z,AIN,BIN,A,NA,B,NB,NOUT,RMAX,VMAX)
C  J.C. NASH JULY 1978, APRIL 1989
C  COMPUTES RESIDUALS AND INNER PRODUCTS
C  R = (A - Z(J)*B)*V(.,J)
C  AIN AND BIN ARE NAMES OF MATRIX CALCULATING ROUTINES FOR A AND B
C  WHOSE FIRST DIMENSIONS ARE NA AND NB RESP.
C  RMAX AND VMAX ARE MAX ABS RESIDUAL AND INNER PRODUCT RESP.

```

C

```

INTEGER N,NV,NA,NB,NOUT,I,J,K,RPOSI,RPOSJ,VPOSI,VPOSJ,I1,N1
REAL V(NV,N),A(NA,N),B(NB,N),Z(N),RMAX,VMAX
DOUBLE PRECISION ACC,TACC,DABS,DBLE
CALL AIN(N,N,A,NA)
CALL BIN(N,N,B,NB)
N1=N-1
TACC=0.0
RPOSI=1
RPOSJ=1
DO 20 I=1,N
  DO 15 J=1,N
    ACC=0.0
    DO 10 K=1,N
      ACC=ACC+DBLE(V(K,J))*(A(I,K)-Z(J)*B(I,K))
10    CONTINUE
      IF(DABS(ACC).LE.TACC)GOTO 15
      TACC=DABS(ACC)
      RPOSI=I
      RPOSJ=J
15    CONTINUE
20  CONTINUE
  RMAX=TACC
  IF(NOUT.GT.0)WRITE(NOUT,951)RMAX,RPOSI,RPOSJ
951 FORMAT(' MAX. ABS. RESIDUAL=',1PE16.8,' POSN',2I4)
  VPOSI=0
  VPOSJ=0
  TACC=0.0
  IF(N.EQ.1)GOTO 45
  DO 40 I=1,N1
    I1=I+1
    DO 35 J=I1,N
      ACC=0.0
      DO 30 K=1,N
        ACC=ACC+DBLE(V(K,I))*V(K,J)
30      CONTINUE
      IF(DABS(ACC).LE.TACC)GOTO 35
      TACC=DABS(ACC)
      VPOSI=I
      VPOSJ=J
35    CONTINUE
40  CONTINUE
  VMAX=TACC
  IF(NOUT.GT.0)WRITE(NOUT,952)VMAX,VPOSI,VPOSJ
952 FORMAT(' MAX. ABS. INNER PRODUCT=',1PE16.8,' POSN',2I4)
  45 IF(NOUT.LE.0)RETURN
  DO 50 J=1,N
    WRITE(NOUT,953)J,Z(J)
953 FORMAT(' EIGENVALUE',I3,'=',1PE16.8)
    WRITE(NOUT,954)(V(K,J),K=1,N)
954 FORMAT(1H ,5E16.8)
  50 CONTINUE
  RETURN

```



```

        END
        SUBROUTINE FRANKM(M,N,A,NA)
C   J.C. NASH    JULY 1978, APRIL 1989
        INTEGER M,N,NA,I,J
C   INPUTS FRANK MATRIX M BY N INTO A
        REAL A(NA,N)
        DO 20 I=1,M
            DO 10 J=1,N
                A(I,J)=AMINO(I,J)
10      CONTINUE
20     CONTINUE
        RETURN
        END

```

Example output

```

## #!/bin/bash
gfortran ../fortran/dr13.f
mv ./a.out ../fortran/dr13.run
../fortran/dr13.run < ../fortran/dr13.in

## ORDER N= 2
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 0 ROTATIONS SKIPPED
## AT SWEEP 3 1 ROTATIONS SKIPPED
## CONVERGED IN 3 SWEEPS
## MAX. ABS. RESIDUAL= 1.47663954E-07 POSN 1 1
## MAX. ABS. INNER PRODUCT= 0.00000000E+00 POSN 0 0
## EIGENVALUE 1= 2.61803412E+00
## 0.52573115E+00 0.85065079E+00
## EIGENVALUE 2= 3.81966025E-01
## -0.85065079E+00 0.52573115E+00
## ORDER N= 4
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 0 ROTATIONS SKIPPED
## AT SWEEP 3 1 ROTATIONS SKIPPED
## AT SWEEP 4 6 ROTATIONS SKIPPED
## CONVERGED IN 4 SWEEPS
## MAX. ABS. RESIDUAL= 6.81894505E-07 POSN 3 1
## MAX. ABS. INNER PRODUCT= 4.60000820E-08 POSN 1 3
## EIGENVALUE 1= 8.29086018E+00
## 0.22801343E+00 0.42852512E+00 0.57735032E+00 0.65653849E+00
## EIGENVALUE 2= 1.00000048E+00
## -0.57735056E+00 -0.57735002E+00 0.66493286E-07 0.57735020E+00
## EIGENVALUE 3= 4.26022291E-01
## 0.65653813E+00 -0.22801332E+00 -0.57735056E+00 0.42852539E+00
## EIGENVALUE 4= 2.83118486E-01
## -0.42852521E+00 0.65653872E+00 -0.57735002E+00 0.22801307E+00
## ORDER N= 4
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 0 ROTATIONS SKIPPED
## AT SWEEP 3 1 ROTATIONS SKIPPED
## AT SWEEP 4 6 ROTATIONS SKIPPED
## CONVERGED IN 4 SWEEPS

```

```

## MAX. ABS. RESIDUAL= 6.81894505E-07 POSN 3 1
## MAX. ABS. INNER PRODUCT= 4.60000820E-08 POSN 1 3
## EIGENVALUE 1= 8.29086018E+00
## 0.22801343E+00 0.42852512E+00 0.57735032E+00 0.65653849E+00
## EIGENVALUE 2= 1.00000048E+00
## -0.57735056E+00 -0.57735002E+00 0.66493286E-07 0.57735020E+00
## EIGENVALUE 3= 4.26022291E-01
## 0.65653813E+00 -0.22801332E+00 -0.57735056E+00 0.42852539E+00
## EIGENVALUE 4= 2.83118486E-01
## -0.42852521E+00 0.65653872E+00 -0.57735002E+00 0.22801307E+00
## ORDER N= 10
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 0 ROTATIONS SKIPPED
## AT SWEEP 3 0 ROTATIONS SKIPPED
## AT SWEEP 4 32 ROTATIONS SKIPPED
## AT SWEEP 5 44 ROTATIONS SKIPPED
## AT SWEEP 6 42 ROTATIONS SKIPPED
## AT SWEEP 7 45 ROTATIONS SKIPPED
## CONVERGED IN 7 SWEEPS
## MAX. ABS. RESIDUAL= 2.39280362E-05 POSN 9 1
## MAX. ABS. INNER PRODUCT= 6.23372785E-08 POSN 6 10
## EIGENVALUE 1= 4.47660294E+01
## 0.65047376E-01 0.12864168E+00 0.18936241E+00 0.24585304E+00 0.29685175E+00
## 0.34121934E+00 0.37796459E+00 0.40626666E+00 0.42549327E+00 0.43521538E+00
## EIGENVALUE 2= 5.04890442E+00
## -0.18936226E+00 -0.34121895E+00 -0.42549327E+00 -0.42549345E+00 -0.34121940E+00
## -0.18936238E+00 -0.18430426E-06 0.18936227E+00 0.34121925E+00 0.42549381E+00
## EIGENVALUE 3= 1.87301636E+00
## 0.29685244E+00 0.43521363E+00 0.34121892E+00 0.65048993E-01 -0.24585134E+00
## -0.42549297E+00 -0.37796640E+00 -0.12864257E+00 0.18936226E+00 0.40626761E+00
## EIGENVALUE 4= 9.99992371E-01
## -0.37796077E+00 -0.37796682E+00 -0.31607331E-05 0.37796402E+00 0.37796602E+00
## 0.20208058E-05 -0.37796175E+00 -0.37796679E+00 -0.16900430E-05 0.37796503E+00
## EIGENVALUE 5= 6.43104553E-01
## 0.42549762E+00 0.18936004E+00 -0.34121791E+00 -0.34121671E+00 0.18935442E+00
## 0.42549407E+00 0.89485920E-05 -0.42549804E+00 -0.18936114E+00 0.34121749E+00
## EIGENVALUE 6= 4.65229034E-01
## -0.43522137E+00 0.65052554E-01 0.42549083E+00 -0.12863764E+00 -0.40626609E+00
## 0.18935713E+00 0.37796399E+00 -0.24584912E+00 -0.34122151E+00 0.29685244E+00
## EIGENVALUE 7= 3.66199493E-01
## 0.40627682E+00 -0.29686981E+00 -0.18934317E+00 0.43520308E+00 -0.12863609E+00
## -0.34122577E+00 0.37796903E+00 0.65047354E-01 -0.42548791E+00 0.24584727E+00
## EIGENVALUE 8= 3.07968140E-01
## -0.34119982E+00 0.42547908E+00 -0.18935996E+00 -0.18936360E+00 0.42549238E+00
## -0.34120587E+00 -0.21800142E-04 0.34124032E+00 -0.42551416E+00 0.18937302E+00
## EIGENVALUE 9= 2.73780823E-01
## 0.24583328E+00 -0.40622735E+00 0.42543337E+00 -0.29676920E+00 0.64941816E-01
## 0.18947297E+00 -0.37804705E+00 0.43525901E+00 -0.34123680E+00 0.12864587E+00
## EIGENVALUE 10= 2.55672455E-01
## -0.12867406E+00 0.24592136E+00 -0.34131119E+00 0.40634301E+00 -0.43523723E+00
## 0.42545170E+00 -0.37787846E+00 0.29675686E+00 -0.18929419E+00 0.65023489E-01
## ORDER N= 1
## CONVERGED IN 0 SWEEPS
## MAX. ABS. RESIDUAL= 0.00000000E+00 POSN 1 1

```

```
## EIGENVALUE 1= 1.00000000E+00
## 0.10000000E+01
## ORDER N= 0
```

BASIC

Listing

```
10 PRINT "A13 EIGENSOLUTIONS OF A SYMMETRIC MATRIX VIA SVD"
20 LET N9=20
30 DIM A(N9,N9),V(N9,N9),B(N9,N9),D(N9),Z(N9)
40 PRINT "ORDER OF MATRIX: ";
50 READ N
55 PRINT N
60 IF (N <= 0) THEN QUIT
70 LET M=N
80 GOSUB 1500: REM BUILD FRANK MATRIX N BY N
100 GOSUB 3000
110 FOR I=1 TO N
120   PRINT "EV(";I;")=";D(I);"      RQ=";Z(I)
130   FOR J=1 TO N
140     PRINT V(J,I);" ";
150   NEXT J
155   PRINT
160 NEXT I
170 PRINT
200 GOTO 40
300 DATA 2, 4, 10, 1, 0
1500 REM PREPARE FRANK MATRIX IN A
1510 FOR I=1 TO M
1530 FOR J=1 TO N
1540 IF (I <= J) THEN LET A(I,J)=I ELSE LET A(I,J)=J
1545 LET B(I,J)=A(I,J)
1550 NEXT J
1560 NEXT I
1570 RETURN
3000 PRINT "SMEV.NJ ALG 13 DEC 7 78"
3002 LET E1=1E-7
3004 IF (N > 1) THEN GOTO 3020
3006 LET D(1)=A(1,1)
3008 LET V(1,1)=1
3010 LET Z(1)=D(1)
3012 RETURN
3014 REM END SPECIAL CASE N=1
3018 REM DIM A(N,N),V(N,N),B(N,N) (FOR RAYLEIGH QUOTIENT)
3020 LET H=1E+38: REM BIG NUMBER
3025 FOR I=1 TO N
3030   LET V1=A(I,I)
3035   FOR J=1 TO N
3040     LET B(I,J)=A(I,J)
3045     IF I=J THEN GOTO 3055
3050     LET V1=V1-ABS(A(I,J))
3055   NEXT J
3060   IF V1>=H THEN GOTO 3070
```

```

3065   LET H=V1
3070 NEXT I
3075 IF H<E1 THEN GOTO 3090
3080 LET H=0
3085 GOTO 3120
3090 LET H=H-SQR(E1)
3095 FOR I=1 TO N
3100   LET A(I,I)=A(I,I)-H
3105 NEXT I
3110 PRINT
3115 PRINT "SCALING BY SUBTRACTION OF",H
3120 LET I9=0
3125 LET N2=N*(N-1)/2
3130 LET N1=N-1
3135 LET N9=N2
3140 LET I9=I9+1
3145 LET N9=0
3150 IF I9<=30 THEN GOTO 3170
3155 PRINT
3160 PRINT "NON-",
3165 GOTO 3355
3170 FOR J=1 TO N1
3175   LET J1=J+1
3180   FOR K=J1 TO N
3185     LET P=0
3190     LET R=0
3195     LET Q=0
3200     FOR I=1 TO N
3205       LET P=P+A(I,J)*A(I,K)
3210       LET Q=Q+A(I,J)*A(I,J)
3215       LET R=R+A(I,K)*A(I,K)
3220     NEXT I
3225     IF 1+ABS(P/SQR(Q*R))>1 THEN GOTO 3235
3230     IF Q>=R THEN GOTO 3320
3235     LET Q=Q-R
3240     LET V1=SQR(4*P*P+Q*Q)
3245     IF V1=0 THEN GOTO 3320
3250     IF Q<0 THEN GOTO 3270
3255     LET C=SQR((V1+Q)/(2*V1))
3260     LET S=P/(V1*C)
3265     GOTO 3290
3270     LET S=SQR((V1-Q)/(2*V1))
3275     IF P>0 THEN GOTO 3285
3280     LET S=-S
3285     LET C=P/(V1*S)
3290     FOR I=1 TO N
3295       LET V1=A(I,J)
3300       LET A(I,J)=V1*C+A(I,K)*S
3305       LET A(I,K)=-V1*S+A(I,K)*C
3310     NEXT I
3315     GOTO 3325
3320     LET N9=N9+1
3325   NEXT K

```

```

3330 NEXT J
3335 IF N9=N2 THEN GOTO 3350
3340 PRINT "SWEEP",I9,"  ",N9,"SMALL P"
3345 GOTO 3140
3350 PRINT
3355 PRINT "CONVERGENCE AT SWEEP",I9
3360 LET V1=0
3365 LET C=0
3370 FOR J=1 TO N
3375   LET Q=0
3380   FOR I=1 TO N
3385     LET Q=Q+A(I,J)^2
3390   NEXT I
3395   LET Q=SQR(Q)
3400   FOR I=1 TO N
3405     LET V(I,J)=A(I,J)/Q
3410   NEXT I
3415   LET Q=Q+H
3420   GOSUB 3440
3425   LET D(J)=Q
3430 NEXT J
3435 RETURN
3440 LET Q=0
3445 FOR I=1 TO N
3450   FOR K=1 TO N
3455     LET Q=Q+V(I,J)*B(I,K)*V(K,J)
3460   NEXT K
3465 NEXT I
3470 LET Z(J)=Q
3475 RETURN

```

Example output

```

bwbasic ../BASIC/a13.bas >../BASIC/a13.out
# echo "done"

```

Bywater BASIC Interpreter/Shell, version 2.20 patch level 2

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A13 EIGENSOLUTIONS OF A SYMMETRIC MATRIX VIA SVD
ORDER OF MATRIX: 2
SMEV.NJ ALG 13 DEC 7 78

SCALING BY SUBTRACTION OF -0.0003162
SWEEP 1 0 SMALL P

CONVERGENCE AT SWEEP 2
EV(1)= 2.6180340 RQ= 2.6180340
0.5257311 0.8506508
EV(2)= 0.381966 RQ= 0.381966

-0.8506508 0.5257311

ORDER OF MATRIX: 4

SMEV.NJ ALG 13 DEC 7 78

SCALING BY SUBTRACTION OF -3.0003162

SWEEP	1	0	SMALL P
SWEEP	2	0	SMALL P
SWEEP	3	0	SMALL P
SWEEP	4	1	SMALL P

CONVERGENCE AT SWEEP 5

EV(1)= 8.2908594 RQ= 8.2908594

0.2280134 0.428525 0.5773503 0.6565385

EV(2)= 1 RQ= 1

-0.5773503 -0.5773503 0 0.5773503

EV(3)= 0.426022 RQ= 0.426022

0.6565385 -0.2280134 -0.5773503 0.428525

EV(4)= 0.2831186 RQ= 0.2831186

-0.428525 0.6565385 -0.5773503 0.2280134

ORDER OF MATRIX: 10

SMEV.NJ ALG 13 DEC 7 78

SCALING BY SUBTRACTION OF -36.0003162

SWEEP	1	0	SMALL P
SWEEP	2	0	SMALL P
SWEEP	3	0	SMALL P
SWEEP	4	0	SMALL P
SWEEP	5	25	SMALL P

CONVERGENCE AT SWEEP 6

EV(1)= 44.7660687 RQ= 44.7660687

0.0650474 0.1286417 0.1893624 0.245853 0.2968517 0.3412192 0.3779645 0.4062666 0.4254934 0.4352154

EV(2)= 5.0489173 RQ= 5.0489173

-0.1893624 -0.3412192 -0.4254934 -0.4254934 -0.3412192 -0.1893624 -0 0.1893624 0.3412192 0.4254934

EV(3)= 1.873023 RQ= 1.873023

0.2968517 0.4352154 0.3412192 0.0650474 -0.245853 -0.4254934 -0.3779645 -0.1286417 0.1893624 0.4062666

EV(4)= 1 RQ= 1

-0.3779645 -0.3779645 -0 0.3779645 0.3779645 0 -0.3779645 -0.3779645 0 0.3779645

EV(5)= 0.6431041 RQ= 0.6431041

0.4254934 0.1893624 -0.3412192 -0.3412192 0.1893624 0.4254934 0 -0.4254934 -0.1893624 0.3412192

EV(6)= 0.465233 RQ= 0.465233

-0.4352154 0.0650474 0.4254934 -0.1286417 -0.4062666 0.1893624 0.3779645 -0.245853 -0.3412192 0.2968517

EV(7)= 0.3662089 RQ= 0.3662089

0.4062666 -0.2968517 -0.1893624 0.4352154 -0.1286417 -0.3412192 0.3779645 0.0650474 -0.4254934 0.245853

```

EV( 8)= 0.3079785    RQ= 0.3079785
-0.3412192  0.4254934 -0.1893624 -0.1893624  0.4254934 -0.3412192 -0  0.34
12192 -0.4254934  0.1893624
EV( 9)= 0.2737868    RQ= 0.2737868
0.245853 -0.4062666  0.4254934 -0.2968517  0.0650474  0.1893624 -0.3779645
0.4352154 -0.3412192  0.1286417
EV( 10)= 0.2556796    RQ= 0.2556796
-0.1286417  0.245853 -0.3412192  0.4062666 -0.4352154  0.4254934 -0.3779645
0.2968517 -0.1893624  0.0650474

ORDER OF MATRIX:  1
SMEV.NJ ALG 13 DEC 7 78
EV( 1)= 1    RQ= 1
1

ORDER OF MATRIX:  0

```

Pascal

Listing

```

Program dr13(input,output);
{dr13.pas == run Nash svd for eigenvalue computations (Alg13)}

    Copyright 1988 J.C.Nash
}
{constype.def ==
This file contains various definitions and type statements which are
used throughout the collection of "Compact Numerical Methods". In many
cases not all definitions are needed, and users with very tight memory
constraints may wish to remove some of the lines of this file when
compiling certain programs.

Modified for Turbo Pascal 5.0

    Copyright 1988, 1990 J.C.Nash
}

const
  big = 1.0E+35;    {a very large number}
  Maxconst = 25;    {Maximum number of constants in data record}
  Maxobs = 100;     {Maximum number of observations in data record}
  Maxparm = 25;     {Maximum number of parameters to adjust}
  Maxvars = 10;     {Maximum number of variables in data record}
  acctol = 0.0001;  {acceptable point tolerance for minimisation codes}
  maxm = 20;        {Maximum number or rows in a matrix}
  maxn = 20;        {Maximum number of columns in a matrix}
  maxmn = 40;       {maxn+maxm, the number of rows in a working array}
  maxsym = 210;     {maximum number of elements of a symmetric matrix
                    which need to be stored = maxm * (maxm + 1)/2 }
  reltest = 10.0;   {a relative size used to check equality of numbers.
                    Numbers x and y are considered equal if the
                    floating-point representation of reltest*x equals

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        that of reltest+y.}
stepredn = 0.2;   {factor to reduce stepsize in line search}
yearwrit = 1990; {year in which file was written}

type
  str2 = string[2];
  rmatrix = array[1..maxm, 1..maxn] of real; {a real matrix}
  wmatrix = array[1..maxmn, 1..maxn] of real; {a working array, formed
        as one real matrix stacked on another}
  smatvec = array[1..maxsym] of real; {a vector to store a symmetric matrix
        as the row-wise expansion of its lower triangle}
  rvector = array[1..maxm] of real; {a real vector. We will use vectors
        of m elements always. While this is NOT space efficient,
        it simplifies program codes.}
  cgmethodtype= (Fletcher_Reeves,Polak_Ribiere,Beale_Sorenson);
  {three possible forms of the conjugate gradients updating formulae}
  probdata = record
    m      : integer; {number of observations}
    nvar   : integer; {number of variables}
    nconst : integer; {number of constants}
    vconst : array[1..Maxconst] of real;
    Ydata  : array[1..Maxobs, 1..Maxvars] of real;
    nlls   : boolean; {true if problem is nonlinear least squares}
  end;

{
  NOTE: Pascal does not let us define the work-space for the function
  within the user-defined code. This is a weakness of Pascal for this
  type of work.
}

var {global definitions}
  banner      : string[80]; {program name and description}

function calceps:real;
{calceps.pas ==
  This function returns the machine EPSILON or floating point tolerance,
  the smallest positive real number such that 1.0 + EPSILON > 1.0.
  EPSILON is needed to set various tolerances for different algorithms.
  While it could be entered as a constant, I prefer to calculate it, since
  users tend to move software between machines without paying attention to
  the computing environment. Note that more complete routines exist.
}
var
  e,e0: real;
  i: integer;
begin {calculate machine epsilon}
  e0 := 1; i:=0;
  repeat
    e0 := e0/2; e := 1+e0; i := i+1;
  until (e=1.0) or (i=50); {note safety check}
  e0 := e0*2;
{ Writeln('Machine EPSILON =',e0);}
  calceps:=e0;

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end; {calceps}

function resids(nRow, nCol: integer; A : rmatrix;
               Y: rvector; Bvec : rvector):real;
{resids.pas
 == Computes residuals and , if print is TRUE, displays them 7
 per line for the linear least squares problem. The sum of
 squared residuals is returned.

 residual vector = A * Bvec - Y
}
var
i, j: integer;
t1, ss : real;

begin
  writeln('Residuals');
  ss:=0.0;
  for i:=1 to nRow do
    begin
      t1:=-Y[i]; {note form of residual is residual = A * B - Y }
      for j:=1 to nCol do
        t1:=t1+A[i,j]*Bvec[j];
        ss:=ss+t1*t1;
        write(t1:10, ' ');
        if (i = 7 * (i div 7)) and (i<nRow) then writeln;
      end; {loop on i}
      writeln;
      writeln('Sum of squared residuals =',ss);
      resids:=ss
    end; {resids.pas == residual calculation for linear least squares}

procedure NashSVD(nRow, nCol: integer;
                 var W: wmatrix;
                 var Z: rvector);

var
  i, j, k, EstColRank, RotCount, SweepCount, slimit : integer;
  eps, e2, tol, vt, p, x0, y0, q, r, c0, s0, d1, d2 : real;

procedure rotate;
var
  ii : integer;

begin
  for ii := 1 to nRow+nCol do
    begin
      D1 := W[ii,j]; D2 := W[ii,k];
      W[ii,j] := D1*c0+D2*s0; W[ii,k] := -D1*s0+D2*c0
    end;
  end;

begin

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writeln('alg01.pas -- NashSVD');
eps := Calceps;
slimit := nCol div 4; if slimit<6 then slimit := 6;

SweepCount := 0;
e2 := 10.0*nRow*eps*eps;
tol := eps*0.1;

EstColRank := nCol; ;

for i := 1 to nCol do
begin
for j := 1 to nCol do
W[nRow+i,j] := 0.0;
W[nRow+i,i] := 1.0;
end;

repeat
RotCount := EstColRank*(EstColRank-1) div 2;
SweepCount := SweepCount+1;

for j := 1 to EstColRank-1 do
begin
for k := j+1 to EstColRank do
begin
p := 0.0; q := 0.0; r := 0.0;
for i := 1 to nRow do
begin
x0 := W[i,j]; y0 := W[i,k];
p := p+x0*y0; q := q+x0*x0; r := r+y0*y0;
end;
Z[j] := q; Z[k] := r;

if q >= r then
begin
if (q<=e2*Z[1]) or (abs(p)<= tol*q) then RotCount := RotCount-1

else
begin
p := p/q; r := 1-r/q; vt := sqrt(4*p*p + r*r);
c0 := sqrt(0.5*(1+r/vt)); s0 := p/(vt*c0);
rotate;
end
end
else
begin

p := p/r; q := q/r-1; vt := sqrt(4*p*p + q*q);
s0 := sqrt(0.5*(1-q/vt));
if p<0 then s0 := -s0;
c0 := p/(vt*s0);
rotate;
end;
end;

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    end;
end;
writeln('End of Sweep #', SweepCount,
        '- no. of rotations performed =', RotCount);
while (EstColRank >= 3) and (Z[EstColRank] <= Z[1]*tol + tol*tol)
    do EstColRank := EstColRank-1;
until (RotCount=0) or (SweepCount>slimit);
if (SweepCount > slimit) then writeln('**** SWEEP LIMIT EXCEEDED');
end;

Procedure evsvd(n: integer; var A,V : rmatrix; initev: boolean;
               W : wmatrix; var Z: rvector);

var
    i, j: integer;
    shift, t : real ;

begin
    writeln('alg13.pas -- symmetric matrix eigensolutions via svd');
    shift:=0.0;
    for i:=1 to n do
        begin
            t:=A[i,i];
            for j:=1 to n do
                if i<>j then t:=t-abs(A[i,j]);
                if t<shift then shift:=t;
            end;
            shift:=-shift;
            if shift<0.0 then shift:=0.0;
            writeln('Adding a shift of ',shift,' to diagonal of matrix. ');
            for i:=1 to n do
                begin
                    for j:=1 to n do
                        begin
                            W[i,j]:=A[i,j];
                            if i=j then W[i,i]:=A[i,i]+shift;
                            if initev then
                                begin
                                    if i=j then W[i+n,i]:=0.0
                                    else
                                        begin
                                            W[i+n,j]:=0.0;
                                        end;
                                end;
                        end;
                    end;
                end;
            end;
            if (n > 1) then
                NashSVD(n, n, W, Z)
            else
                begin { order 1 matrix }
                    Z[1] := A[1,1]*A[1,1];
                    W[2,1]:= 1.0; {Eigenvector!}
                end;
            end;

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for i:=1 to n do
begin
  Z[i]:=sqrt(Z[i])-shift;
  for j:=1 to n do
    V[i,j]:=W[n+i,j];
  end;
end;

Procedure Frank2(var m, n: integer; var A: rmatrix);
var
  i,j: integer;
begin
  for i:=1 to m do
    begin
      for j:=1 to n do
        begin
          if (i <= j) then
            A[i,j]:=i
          else
            A[i,j]:=j;
          end;
        end;
      end;
    end;

var
  i, j, nRow, nCol : integer;
  A, V, ACOPY : rmatrix;
  Bvec, Y, Z : rvector;
  W : wmatrix; {to store the working array}
  t1: real;
  initev : boolean;

begin
  banner:='dr13.pas -- driver for svd eigensolutions of a symmetric matrix';
  nRow := 1; {To get loop going}
  while (nRow > 0) do
    begin
      write('Order of problem (n): '); readln(nRow);
      if (nRow <= 0) then halt;
      nCol := nRow;
      Frank2(nRow, nCol, A);
      writeln('Initial matrix of order ', nRow);
      for j := 1 to nRow do
        begin
          for i := 1 to nRow do
            begin
              write(A[i,j]:10:5, ' ');
              ACOPY[i,j] := A[i,j];
              W[i,j]:=0.0; {to avoid warning 'uninitialized' from fpc}
              if (7 * (i div 7) = i) and (i<nRow) then
                begin
                  writeln;
                end;
            end;
          end;
        end;
      end;
    end;
  end;

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    end;
    writeln;
end;
initev := true; {Here we want to get the eigenvectors of A, not some
                generalized problem.}
writeln('Calling evsvd');
evsvd( nRow, A, V, initev, W, Z);
for j := 1 to nRow do
begin
    t1 := Z[j];
    writeln;
    writeln('Eigenvalue ',j,' = ',t1);
    for i := 1 to nRow do
    begin
        write(V[i,j]:10:7,' ');
        if (i = 7 * (i div 7)) and (i<nRow) then
        begin
            writeln;
        end;
        Bvec[i] := V[i,j]; {to initialize residual test}
        Y[i] := t1*Bvec[i];
    end;
    writeln;
    t1 := resids(nRow, nCol, ACOPY, Y, Bvec);
end; {loop on solutions j}
end; {main while loop}
end. {dr13.pas}

```

Example output

```

fpc ../Pascal2021/dr13.pas
# copy to run file
mv ../Pascal2021/dr13 ../Pascal2021/dr13.run
../Pascal2021/dr13.run <../Pascal2021/dr13p.in >../Pascal2021/dr13p.out

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr13.pas
## Linking ../Pascal2021/dr13
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 326 lines compiled, 0.1 sec

Order of problem (n): Initial matrix of order 2
  1.00000  1.00000
  1.00000  2.00000
Calling evsvd
alg13.pas -- symmetric matrix eigensolutions via svd
Adding a shift of -0.0000000000000000E+000 to diagonal of matrix.
alg01.pas -- NashSVD
End of Sweep #1- no. of rotations performed =1
End of Sweep #2- no. of rotations performed =0

Eigenvalue 1 = 2.6180339887498945E+000

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0.5257311 0.8506508
Residuals
1.11E-016 4.44E-016
Sum of squared residuals = 2.0954117794933126E-031

Eigenvalue 2 = 3.8196601125010510E-001
-0.8506508 0.5257311
Residuals
0.00E+000 0.00E+000
Sum of squared residuals = 0.0000000000000000E+000
Order of problem (n): Initial matrix of order 4
1.00000 1.00000 1.00000 1.00000
1.00000 2.00000 2.00000 2.00000
1.00000 2.00000 3.00000 3.00000
1.00000 2.00000 3.00000 4.00000
Calling evsvd
alg13.pas -- symmetric matrix eigensolutions via svd
Adding a shift of 3.0000000000000000E+000 to diagonal of matrix.
alg01.pas -- NashSVD
End of Sweep #1- no. of rotations performed =6
End of Sweep #2- no. of rotations performed =6
End of Sweep #3- no. of rotations performed =6
End of Sweep #4- no. of rotations performed =4
End of Sweep #5- no. of rotations performed =0

Eigenvalue 1 = 8.2908593693815913E+000
0.2280134 0.4285251 0.5773503 0.6565385
Residuals
-1.22E-015 2.22E-016 -1.55E-015 -2.22E-015
Sum of squared residuals = 8.8870111353804611E-030

Eigenvalue 2 = 1.0000000000000009E+000
-0.5773503 -0.5773503 0.0000000 0.5773503
Residuals
6.66E-016 4.44E-016 -2.22E-016 -4.44E-016
Sum of squared residuals = 8.8746851837363828E-031

Eigenvalue 3 = 4.2602204776046149E-001
0.6565385 -0.2280134 -0.5773503 0.4285251
Residuals
2.78E-016 -1.11E-016 2.22E-016 6.66E-016
Sum of squared residuals = 5.8240121518270012E-031

Eigenvalue 4 = 2.8311858285794766E-001
-0.4285251 0.6565385 -0.5773503 0.2280134
Residuals
-3.89E-016 8.88E-016 -1.11E-016 5.55E-016
Sum of squared residuals = 1.2603285556070071E-030
Order of problem (n): Initial matrix of order 10
1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
1.00000 1.00000 1.00000
1.00000 2.00000 2.00000 2.00000 2.00000 2.00000 2.00000
2.00000 2.00000 2.00000

```

1.00000	2.00000	3.00000	3.00000	3.00000	3.00000	3.00000
3.00000	3.00000	3.00000				
1.00000	2.00000	3.00000	4.00000	4.00000	4.00000	4.00000
4.00000	4.00000	4.00000				
1.00000	2.00000	3.00000	4.00000	5.00000	5.00000	5.00000
5.00000	5.00000	5.00000				
1.00000	2.00000	3.00000	4.00000	5.00000	6.00000	6.00000
6.00000	6.00000	6.00000				
1.00000	2.00000	3.00000	4.00000	5.00000	6.00000	7.00000
7.00000	7.00000	7.00000				
1.00000	2.00000	3.00000	4.00000	5.00000	6.00000	7.00000
8.00000	8.00000	8.00000				
1.00000	2.00000	3.00000	4.00000	5.00000	6.00000	7.00000
8.00000	9.00000	9.00000				
1.00000	2.00000	3.00000	4.00000	5.00000	6.00000	7.00000
8.00000	9.00000	10.00000				

Calling evsvd

alg13.pas -- symmetric matrix eigensolutions via svd

Adding a shift of 3.600000000000000E+001 to diagonal of matrix.

alg01.pas -- NashSVD

End of Sweep #1- no. of rotations performed =45

End of Sweep #2- no. of rotations performed =45

End of Sweep #3- no. of rotations performed =45

End of Sweep #4- no. of rotations performed =45

End of Sweep #5- no. of rotations performed =16

End of Sweep #6- no. of rotations performed =0

Eigenvalue 1 = 4.4766068652715035E+001

0.0650474	0.1286417	0.1893624	0.2458530	0.2968517	0.3412192	0.3779645
0.4062666	0.4254934	0.4352154				

Residuals

4.61E-015	3.89E-015	1.11E-015	6.00E-015	9.77E-015	4.00E-015	8.88E-016
1.33E-015	-7.99E-015	1.78E-015				

Sum of squared residuals = 2.5454630888977219E-028

Eigenvalue 2 = 5.0489173395222977E+000

-0.1893624	-0.3412192	-0.4254934	-0.4254934	-0.3412192	-0.1893624	-0.0000000
0.1893624	0.3412192	0.4254934				

Residuals

-2.05E-015	-7.66E-015	-5.33E-015	1.55E-015	-4.44E-015	-3.55E-015	-8.88E-016
2.22E-015	1.78E-015	1.78E-015				

Sum of squared residuals = 1.3809071775652032E-028

Eigenvalue 3 = 1.8730230604248987E+000

0.2968517	0.4352154	0.3412192	0.0650474	-0.2458530	-0.4254934	-0.3779645
-0.1286417	0.1893624	0.4062666				

Residuals

9.55E-015	7.55E-015	3.11E-015	-2.66E-015	0.00E+000	-5.33E-015	-9.33E-015
8.88E-016	-8.88E-016	-8.88E-016				

Sum of squared residuals = 2.8265872310200379E-028

Eigenvalue 4 = 9.999999999999289E-001

-0.3779645	-0.3779645	-0.0000000	0.3779645	0.3779645	0.0000000	-0.3779645
------------	------------	------------	-----------	-----------	-----------	------------

```

-0.3779645 -0.0000000 0.3779645
Residuals
-6.61E-015 -4.88E-015 -2.44E-015 2.66E-015 1.78E-015 8.88E-016 -4.44E-015
4.44E-016 8.88E-016 -1.33E-015
Sum of squared residuals = 1.0699234175851075E-028

Eigenvalue 5 = 6.4310413210777284E-001
0.4254934 0.1893624 -0.3412192 -0.3412192 0.1893624 0.4254934 -0.0000000
-0.4254934 -0.1893624 0.3412192
Residuals
8.55E-015 1.18E-014 -6.88E-015 -1.33E-015 3.11E-015 7.11E-015 4.44E-015
-7.99E-015 -8.88E-016 5.33E-015
Sum of squared residuals = 4.3368860859689532E-028

Eigenvalue 6 = 4.6523308780856354E-001
-0.4352154 0.0650474 0.4254934 -0.1286417 -0.4062666 0.1893624 0.3779645
-0.2458530 -0.3412192 0.2968517
Residuals
-2.89E-015 -2.89E-015 1.55E-015 -6.22E-015 1.11E-015 3.11E-015 -1.33E-015
-3.11E-015 -1.33E-015 -7.99E-015
Sum of squared residuals = 1.4574205223958193E-028

Eigenvalue 7 = 3.6620887461579343E-001
0.4062666 -0.2968517 -0.1893624 0.4352154 -0.1286417 -0.3412192 0.3779645
0.0650474 -0.4254934 0.2458530
Residuals
3.69E-015 -2.83E-015 -1.08E-014 3.33E-016 -4.22E-015 -6.88E-015 -1.78E-015
-5.11E-015 -2.22E-015 -6.66E-015
Sum of squared residuals = 2.8144846872495085E-028

Eigenvalue 8 = 3.0797852836987971E-001
-0.3412192 0.4254934 -0.1893624 -0.1893624 0.4254934 -0.3412192 0.0000000
0.3412192 -0.4254934 0.1893624
Residuals
-5.61E-015 1.24E-014 -1.44E-015 -3.22E-015 1.39E-014 -3.77E-015 -1.33E-015
1.24E-014 -7.77E-015 7.77E-015
Sum of squared residuals = 6.8252800187545925E-028

Eigenvalue 9 = 2.7378676163923643E-001
0.2458530 -0.4062666 0.4254934 -0.2968517 0.0650474 0.1893624 -0.3779645
0.4352154 -0.3412192 0.1286417
Residuals
-5.30E-015 -5.55E-017 7.33E-015 -3.66E-015 -2.33E-015 -3.33E-015 -8.44E-015
6.00E-015 -1.78E-015 -1.11E-015
Sum of squared residuals = 2.2327613994072327E-028

Eigenvalue 10 = 2.5567956279643766E-001
-0.1286417 0.2458530 -0.3412192 0.4062666 -0.4352154 0.4254934 -0.3779645
0.2968517 -0.1893624 0.0650474
Residuals
1.18E-015 -2.25E-015 -1.67E-015 -5.00E-016 4.44E-015 -4.44E-016 -6.11E-016
9.99E-016 9.99E-016 2.66E-015
Sum of squared residuals = 3.8856984778973554E-029

```



```
Order of problem (n): Initial matrix of order 1
1.00000
Calling evsvd
alg13.pas -- symmetric matrix eigensolutions via svd
Adding a shift of -0.000000000000000E+000 to diagonal of matrix.

Eigenvalue 1 = 1.000000000000000E+000
1.0000000
Residuals
0.00E+000
Sum of squared residuals = 0.000000000000000E+000
Order of problem (n):
```

Algorithms 14 and 15 - Generalized symmetric eigenproblem

We aim to solve the generalized symmetric eigenproblem

$$Ax = eBx$$

for x and e , where symmetric matrices A and B and B is positive definite.

Fortran

Listing

```
C&&& A14-15
C TEST ALG. 15 JULY 1978
C J.C. NASH JULY 1978, APRIL 1989
    LOGICAL FAIL
    INTEGER N,ND,I,NOUT,NIN
    REAL A(20,20),B(20,20),AT(20,20),Z(20),V(20,20),RMAX,VMAX
    EXTERNAL FRANKM,UNITM
    ND=20
C I/O CHANNELS
    NIN=5
    NOUT=6
    1 READ(NIN,900)N
    900 FORMAT(I4)
    WRITE(NOUT,901)N
    901 FORMAT(' ORDER N=',I4)
    IF(N.LE.0)STOP
    ISWP=30
    FAIL=.FALSE.
    CALL UNITM(N,N,A,ND)
    CALL FRANKM(N,N,B,ND)
    CALL A15GSE(N,A,ND,B,ND,V,ND,FAIL,ISWP,NOUT)
    IF(FAIL)WRITE(NOUT,904)
    904 FORMAT(' FAILURE SET')
    DO 20 I=1,N
        Z(I)=A(I,I)
    20 CONTINUE
    CALL EVT(N,V,ND,Z,UNITM,FRANKM,AT,ND,B,ND,NOUT,RMAX,VMAX)
    GOTO 1
    END
    SUBROUTINE A14JE(N,A,NA,V,NV,ISWP,IPR,SETV,COMV)
C ALGORITHM 14 JACOBI EIGENVALUES AND EIGENVECTORS OF REAL SYMMETRIC
C MATRIX
C J.C. NASH JULY 1978, FEBRUARY 1980, APRIL 1989
C N = ORDER OF PROBLEM
C A = ARRAY CONTAINING MATRIX -- MUST BE SYMMETRIC
C NA = FIRST DIMENSION OF A
C V = ARRAY INTO WHICH VECTORS COMPUTED
C NV = FIRST DIMENSION OF V
C ISWP = SWEEP LIMIT (INPUT). SWEEP COUNT (OUTPUT)
C IPR = PRINT CHANNEL. PRINTING ONLY IF IPR.GT.0
C SETV = LOGICAL SWITCH TO SET V INITIALLY TO IDENTITY OF ORDER N.
C COMV = LOGICAL SWITCH. IF .TRUE. THEN VECTORS TO BE CALCULATED.
```

```

C  STEP 0
      LOGICAL SETV,COMV
      INTEGER N,NA,NV,IPR,ISWP,LISWP,M,I,J,K,N1,I1
      REAL A(NA,N),V(NV,N),P,Q,T,S,C,FACT
C  FACTOR USED IN TEST AT STEP 7
      FACT=100.0
      N1=N-1
      LISWP=ISWP
      ISWP=0
C  EIGENVALUES LEFT IN DIAGONAL ELEMENTS OF A.
      IF(.NOT.COMV)GOTO 10
      IF(.NOT.SETV)GOTO 10
      DO 5 I=1,N
        DO 3 J=1,N
          V(I,J)=0.0
        3  CONTINUE
          V(I,I)=1.0
      5  CONTINUE
C  STEP 1
      10  ISWP=ISWP+1
          IF(ISWP.GT.LISWP)RETURN
          M=0
C  STEP 2
          IF(N.EQ.1)RETURN
          DO 160 I=1,N1
C  STEP 3
            I1=I+1
            DO 150 J=I1,N
C  STEP 4
              P=0.5*(A(I,J)+A(J,I))
              Q=A(I,I)-A(J,J)
              T=SQRT(4.0*P*P+Q*Q)
C  STEP 5
              IF(T.EQ.0.0)GOTO 110
C  STEP 6
              IF(Q.LT.0.0)GOTO 90
C  STEP 7
              IF(ABS(A(I,I)).LT.ABS(A(I,I))+FACT*ABS(P))GOTO 80
              IF(ABS(A(J,J)).EQ.ABS(A(J,J))+FACT*ABS(P))GOTO 110
C  STEP 8
              80  C=SQRT((T+Q)/(2.0*T))
                  S=P/(T*C)
                  GOTO 100
C  STEP 9
              90  S=SQRT((T-Q)/(2.0*T))
                  IF(P.LT.0.0)S=-S
                  C=P/(T*S)
C  STEP 10
              100  IF(1.0.LT.1.0+ABS(S))GOTO 120
C  STEP 11
              110  M=M+1
                  GOTO 150
C  STEP 12

```

```

120      DO 125 K=1,N
          Q=A(I,K)
          A(I,K)=C*Q+S*A(J,K)
          A(J,K)=-S*Q+C*A(J,K)
125      CONTINUE
C  STEP 13
      DO 135 K=1,N
          Q=A(K,I)
          A(K,I)=C*Q+S*A(K,J)
          A(K,J)=-S*Q+C*A(K,J)
135      CONTINUE
          IF(.NOT.COMV)GOTO 150
C  STEP 14
      DO 145 K=1,N
          Q=V(K,I)
          V(K,I)=C*Q+S*V(K,J)
          V(K,J)=-S*Q+C*V(K,J)
145      CONTINUE
C  STEP 15
150      CONTINUE
C  STEP 16
160      CONTINUE
C  STEP 17
      IF(IPR.GT.0)WRITE(IPR,970)ISWP,M
970      FORMAT( 9H AT SWEEP,I4,2X,I4,18H ROTATIONS SKIPPED)
      IF(M.LT.N*(N-1)/2)GOTO 10
      RETURN
      END
      SUBROUTINE A15GSE(N,A,NA,B,NB,V,NV,FAIL,ISWP,IPR)
C  ALGORITHM 15 GENERALISED SYMMETRIC EIGENPROBLEM BY 2 APPLICATIONS
C  OF JACOBI ALGORITHM 14
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C  N          = ORDER OF PROBLEM
C  A          = A MATRIX OF EIGENPROBLEM. DIAGONAL ELEMENTS BECOME
C  NA         = FIRST DIMENSION OF A
C  B          = B MATRIX OF EIGENPROBLEM, MUST BE POSITIVE DEFINITE
C  NB         = FIRST DIMENSION OF B
C  V          = VECTOR MATRIX. ON OUTPUT COLUMNS ARE EIGENVECTORS
C              EIGENVALUES
C  FAIL       = LOGICAL FLAG SET .TRUE. IF B NOT COMPUTATIONALLY
C              POSITIVE DEFINITE OR IF EITHER APPLICATION OF
C              ALGORITHM 14 TAKES MORE THAN ISWP SWEEPS
C  NV         = FIRST DIMENSION OF V
C  ISWP       = BOUND ON SWEEPS IN ALG. 14.
C  NA,NB,NV ALL .GE. N
C  IPR        = PRINT CHANNEL. IPR.GT.0 FOR PRINTING
C  STEP 0
      LOGICAL FAIL,COMV,SETV
      INTEGER N,NA,NB,NV,STAGE,ISWP,LISWP,I,J,K,M,IPR
      REAL A(NA,N),B(NB,N),V(NV,N),S
      FAIL=.FALSE.
      STAGE=1
      SETV=.TRUE.

```

```

      COMV=.TRUE.
C  STEP 1  INTERCHANGE - NOT GENERALLY EFFICIENT
10  DO 16 I=1,N
      DO 14 J=1,N
        S=A(I,J)
        A(I,J)=B(I,J)
        B(I,J)=S
14    CONTINUE
16  CONTINUE
C  STEP 2
      LISWP=ISWP
      IF(IPR.GT.0)WRITE(IPR,964)STAGE
964  FORMAT( 6H0STAGE,I3)
      CALL A14JE(N,A,NA,V,NV,LISWP,IPR,SETV,COMV)
      IF(LISWP.GE.ISWP)FAIL=.TRUE.
      IF(FAIL)RETURN
C  STEP 3
      IF(STAGE.EQ.2)GOTO 80
C  STEP 4
      STAGE=2
      SETV=.FALSE.
      DO 46 I=1,N
        IF(A(I,I).LE.0.0)FAIL=.TRUE.
        IF(FAIL)RETURN
        S=1.0/SQRT(A(I,I))
        DO 44 J=1,N
          V(J,I)=S*V(J,I)
44    CONTINUE
46  CONTINUE
C  STEP 5
      DO 56 I=1,N
        DO 54 J=1,N
          A(I,J)=B(I,J)
54    CONTINUE
56  CONTINUE
C  STEP 6
      DO 68 I=1,N
        DO 66 J=I,N
          S=0.0
          DO 64 K=1,N
            DO 62 M=1,N
              S=S+V(K,I)*A(K,M)*V(M,J)
62    CONTINUE
64    CONTINUE
          B(I,J)=S
          B(J,I)=S
66    CONTINUE
68  CONTINUE
C  STEP 7
      GOTO 10
80  ISWP=0
      RETURN
      END

```

```

      SUBROUTINE UNITM(M,N,A,NA)
C   PUTS UNIT MATRIX M BY N IN A
C   J.C. NASH   JULY 1978, APRIL 1989
      INTEGER M,N,NA,I,J
      REAL A(NA,N)
      DO 10 I=1,M
        DO 5 J=1,N
          A(I,J)=0.0
          IF(I.EQ.J)A(I,I)=1.0
5      CONTINUE
10     CONTINUE
      RETURN
      END

      SUBROUTINE EVT(N,V,NV,Z,AIN,BIN,A,NA,B,NB,NOUT,RMAX,VMAX)
C   J.C. NASH   JULY 1978, APRIL 1989
C   COMPUTES RESIDUALS AND INNER PRODUCTS
C   R = (A - Z(J)*B)*V(.,J)
C   AIN AND BIN ARE NAMES OF MATRIX CALCULATING ROUTINES FOR A AND B
C   WHOSE FIRST DIMENSIONS ARE NA AND NB RESP.
C   RMAX AND VMAX ARE MAX ABS RESIDUAL AND INNER PRODUCT RESP.
C
      INTEGER N,NV,NA,NB,NOUT,I,J,K,RPOSI,RPOSJ,VPOSI,VPOSJ,I1,N1
      REAL V(NV,N),A(NA,N),B(NB,N),Z(N),RMAX,VMAX
      DOUBLE PRECISION ACC,TACC,DABS,DBLE
      CALL AIN(N,N,A,NA)
      CALL BIN(N,N,B,NB)
      N1=N-1
      TACC=0.0
      RPOSI=1
      RPOSJ=1
      DO 20 I=1,N
        DO 15 J=1,N
          ACC=0.0
          DO 10 K=1,N
            ACC=ACC+DBLE(V(K,J))*(A(I,K)-Z(J)*B(I,K))
10         CONTINUE
          IF(DABS(ACC).LE.TACC)GOTO 15
          TACC=DABS(ACC)
          RPOSI=I
          RPOSJ=J
15        CONTINUE
20      CONTINUE
      RMAX=TACC
      IF(NOUT.GT.0)WRITE(NOUT,951)RMAX,RPOSI,RPOSJ
951  FORMAT(' MAX. ABS. RESIDUAL=',1PE16.8,' POSN',2I4)
      VPOSI=0
      VPOSJ=0
      TACC=0.0
      IF(N.EQ.1)GOTO 45
      DO 40 I=1,N1
        I1=I+1
        DO 35 J=I1,N
          ACC=0.0

```

```

        DO 30 K=1,N
            ACC=ACC+DBLE(V(K,I))*V(K,J)
30      CONTINUE
        IF(DABS(ACC).LE.TACC)GOTO 35
        TACC=DABS(ACC)
        VPOSI=I
        VPOSJ=J
35      CONTINUE
40      CONTINUE
        VMAX=TACC
        IF(NOUT.GT.0)WRITE(NOUT,952)VMAX,VPOSI,VPOSJ
952    FORMAT(' MAX. ABS. INNER PRODUCT=',1PE16.8,' POSN',2I4)
45      IF(NOUT.LE.0)RETURN
        DO 50 J=1,N
            WRITE(NOUT,953)J,Z(J)
953    FORMAT(' EIGENVALUE',I3,'=',1PE16.8)
            WRITE(NOUT,954)(V(K,J),K=1,N)
954    FORMAT(1H ,5E16.8)
50      CONTINUE
        RETURN
        END
        SUBROUTINE FRANKM(M,N,A,NA)
C   J.C. NASH   JULY 1978, APRIL 1989
        INTEGER M,N,NA,I,J
C   INPUTS FRANK MATRIX M BY N INTO A
        REAL A(NA,N)
        DO 20 I=1,M
            DO 10 J=1,N
                A(I,J)=AMINO(I,J)
10          CONTINUE
20        CONTINUE
        RETURN
        END

```

Example output

```

## #!/bin/bash
gfortran ../fortran/dr1415.f
mv ./a.out ../fortran/dr1415.run
# use dr13 here as well as in Alg 13
../fortran/dr1415.run < ../fortran/dr13.in

## ORDER N= 2
## OSTAGE 1
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 1 ROTATIONS SKIPPED
## OSTAGE 2
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 1 ROTATIONS SKIPPED
## MAX. ABS. RESIDUAL= 2.51580275E-07 POSN 2 1
## MAX. ABS. INNER PRODUCT= 7.73007969E-09 POSN 1 2
## EIGENVALUE 1= 2.61803389E+00
## 0.13763819E+01 -0.85065085E+00
## EIGENVALUE 2= 3.81965995E-01

```

```

##      0.32491970E+00  0.52573109E+00
## ORDER N= 4
## OSTAGE 1
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 0 ROTATIONS SKIPPED
## AT SWEEP 3 1 ROTATIONS SKIPPED
## AT SWEEP 4 6 ROTATIONS SKIPPED
## OSTAGE 2
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 5 ROTATIONS SKIPPED
## AT SWEEP 3 6 ROTATIONS SKIPPED
## MAX. ABS. RESIDUAL= 9.88243642E-07 POSN 3 1
## MAX. ABS. INNER PRODUCT= 5.05645765E-08 POSN 1 3
## EIGENVALUE 1= 3.53208756E+00
## -0.80536371E+00 0.12338886E+01 -0.10850633E+01 0.42852503E+00
## EIGENVALUE 2= 2.34729719E+00
## -0.10058755E+01 0.34933683E+00 0.88455212E+00 -0.65653861E+00
## EIGENVALUE 3= 1.00000060E+00
## -0.57735038E+00 -0.57735050E+00 -0.25529275E-07 0.57735038E+00
## EIGENVALUE 4= 1.20614767E-01
## -0.79188228E-01 -0.14882518E+00 -0.20051166E+00 -0.22801344E+00
## ORDER N= 4
## OSTAGE 1
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 0 ROTATIONS SKIPPED
## AT SWEEP 3 1 ROTATIONS SKIPPED
## AT SWEEP 4 6 ROTATIONS SKIPPED
## OSTAGE 2
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 5 ROTATIONS SKIPPED
## AT SWEEP 3 6 ROTATIONS SKIPPED
## MAX. ABS. RESIDUAL= 9.88243642E-07 POSN 3 1
## MAX. ABS. INNER PRODUCT= 5.05645765E-08 POSN 1 3
## EIGENVALUE 1= 3.53208756E+00
## -0.80536371E+00 0.12338886E+01 -0.10850633E+01 0.42852503E+00
## EIGENVALUE 2= 2.34729719E+00
## -0.10058755E+01 0.34933683E+00 0.88455212E+00 -0.65653861E+00
## EIGENVALUE 3= 1.00000060E+00
## -0.57735038E+00 -0.57735050E+00 -0.25529275E-07 0.57735038E+00
## EIGENVALUE 4= 1.20614767E-01
## -0.79188228E-01 -0.14882518E+00 -0.20051166E+00 -0.22801344E+00
## ORDER N= 10
## OSTAGE 1
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 0 ROTATIONS SKIPPED
## AT SWEEP 3 0 ROTATIONS SKIPPED
## AT SWEEP 4 23 ROTATIONS SKIPPED
## AT SWEEP 5 45 ROTATIONS SKIPPED
## OSTAGE 2
## AT SWEEP 1 0 ROTATIONS SKIPPED
## AT SWEEP 2 35 ROTATIONS SKIPPED
## AT SWEEP 3 45 ROTATIONS SKIPPED
## MAX. ABS. RESIDUAL= 7.95809774E-06 POSN 10 1
## MAX. ABS. INNER PRODUCT= 1.70029864E-07 POSN 1 3

```



```

## EIGENVALUE 1= 3.91114664E+00
## 0.25440717E+00 -0.48620966E+00 0.67481190E+00 -0.80345494E+00 0.86070871E+00
## -0.84148449E+00 0.74749005E+00 -0.58707643E+00 0.37449750E+00 -0.12864262E+00
## EIGENVALUE 2= 3.65247846E+00
## -0.46986169E+00 0.77643681E+00 -0.81318295E+00 0.56733066E+00 -0.12432010E+00
## -0.36189401E+00 0.72234160E+00 -0.83175814E+00 0.65211862E+00 -0.24585268E+00
## EIGENVALUE 3= 3.24698114E+00
## -0.61485553E+00 0.76671326E+00 -0.34122097E+00 -0.34121776E+00 0.76671290E+00
## -0.61485648E+00 0.70596684E-09 0.61485595E+00 -0.76671231E+00 0.34121889E+00
## EIGENVALUE 4= 2.73068285E+00
## -0.67134637E+00 0.49054128E+00 0.31291714E+00 -0.71918464E+00 0.21257788E+00
## 0.56385678E+00 -0.62457776E+00 -0.10748890E+00 0.70311815E+00 -0.40626636E+00
## EIGENVALUE 5= 2.14946055E+00
## 0.63807106E+00 -0.95366970E-01 -0.62381732E+00 0.18860267E+00 0.59562886E+00
## -0.27762464E+00 -0.55413532E+00 0.36044526E+00 0.50026351E+00 -0.43521550E+00
## EIGENVALUE 6= 1.55495822E+00
## -0.53058165E+00 -0.23613074E+00 0.42549348E+00 0.42549339E+00 -0.23613124E+00
## -0.53058165E+00 0.14518602E-06 0.53058153E+00 0.23613124E+00 -0.42549354E+00
## EIGENVALUE 7= 1.00000012E+00
## -0.37796488E+00 -0.37796432E+00 0.30240781E-06 0.37796441E+00 0.37796423E+00
## -0.16945556E-08 -0.37796435E+00 -0.37796468E+00 0.11743472E-06 0.37796459E+00
## EIGENVALUE 8= 5.33896327E-01
## -0.21690433E+00 -0.31800413E+00 -0.24932273E+00 -0.47528878E-01 0.17964047E+00
## 0.31090042E+00 0.27617189E+00 0.93996122E-01 -0.13836364E+00 -0.29685175E+00
## EIGENVALUE 9= 1.98062271E-01
## 0.84274180E-01 0.15185684E+00 0.18936239E+00 0.18936241E+00 0.15185687E+00
## 0.84274203E-01 -0.56293572E-07 -0.84274210E-01 -0.15185684E+00 -0.18936238E+00
## EIGENVALUE 10= 2.23383494E-02
## 0.97219953E-02 0.19226812E-01 0.28302142E-01 0.36745246E-01 0.44367522E-01
## 0.50998691E-01 0.56490630E-01 0.60720690E-01 0.63594334E-01 0.65047383E-01
## ORDER N= 1
## OSTAGE 1
## OSTAGE 2
## MAX. ABS. RESIDUAL= 0.00000000E+00 POSN 1 1
## EIGENVALUE 1= 1.00000000E+00
## 0.10000000E+01
## ORDER N= 0
## Note: The following floating-point exceptions are signalling: IEEE_UNDERFLOW_FLAG IEEE_DENORMAL

```

Algorithm 25 – Rayleigh quotient minimization

Fortran

Listing

```
C&&& A25
C TEST ALG 25 USING GRID (5 POINT)
C J.C. NASH JULY 1978, APRIL 1989
  LOGICAL IFR
  INTEGER N,M,NOUT,NIN,KPR,LIMIT,I
  EXTERNAL APR,BPR
C REAL EPS,PO,X(N),S(N),T(N),U(N),V(N),W(N),Y(N),RNORM
  COMMON /GSZ/ M,IFR,R(1600)
  REAL EPS,PO,RNORM,VNORM,RNV
  REAL S(1600),T(1600),U(1600),V(1600),W(1600),X(1600),Y(1600)
C I/O CHANNELS
  NIN=5
  NOUT=6
  1 READ(NIN,900)M,LIMIT
900 FORMAT(2I4)
  N=M*M
  WRITE(NOUT,950)M,N,LIMIT
950 FORMAT(' GRID ORDER',I4,' EQNS ORDER',I5,' LIMIT=',I4)
  IF(M.LE.0)STOP
  IFR=.FALSE.
C IBM MACHINE PRECISION
  EPS=16.0**(-5)
  KPR=LIMIT
  RNORM=1.0/SQRT(FLOAT(N))
  DO 10 I=1,N
    X(I)=RNORM
  10 CONTINUE
  CALL A25RQM(N,X,EPS,KPR,S,T,U,V,W,Y,PO,NOUT,APR,BPR)
  WRITE(NOUT,951)KPR,PO
951 FORMAT(' RETURNED AFTER',I4,' PRODUCTS WITH EV=',1PE16.8)
  DO 20 I=1,N
    R(I)=-PO*X(I)
  20 CONTINUE
  CALL APR(N,X,V)
  RNORM=0.0
  VNORM=0.0
  DO 30 I=1,N
    RNORM=RNORM+(V(I)+R(I))**2
    VNORM=VNORM+X(I)**2
  30 CONTINUE
  RNORM=SQRT(RNORM/N)
  VNORM=SQRT(VNORM/N)
  RNV=RNORM/VNORM
  WRITE(NOUT,952)RNORM,VNORM,RNV
952 FORMAT(' RESIDUAL NORM=',1PE16.8,' /',E16.8,'=',E16.8)
  GOTO 1
  END
  SUBROUTINE BPR(N,X,V)
```

```

C J.C. NASH JULY 1978, APRIL 1989
C UNITM MATRIX * X INTO V
      INTEGER N,I
      REAL X(N),V(N)
      DO 100 I=1,N
        V(I)=X(I)
100 CONTINUE
      RETURN
      END
      SUBROUTINE APR(N,X,V)
C J.C. NASH JULY 1978, APRIL 1989
      LOGICAL IFR
      INTEGER N,I,J,M
      DOUBLE PRECISION S
      REAL X(N),V(N),D,Q
C M BY M GRID OF A GEORGE M=SQRT(N)
      COMMON /GSZ/ M,IFR,R(1600)
C COMMON /GSZ/M
      D=4.0
      Q=-1.0
      DO 100 I=1,N
C NOTE ALL INTEGERS
        J=I/M
        J=M*J
        S=D*X(I)
C SUBTRACT RHS FOR RESIDUAL
        IF(IFR)S=S-R(I)
C LEFT EDGE
        IF(I-J.EQ.1)GOTO 20
        S=S+Q*X(I-1)
C RIGHT EDGE
20 IF(I.GT.J)S=S+Q*X(I+1)
C TOP EDGE
        IF(I.GT.M)S=S+Q*X(I-M)
C BOTTOM EDGE
        IF(I.LE.N-M)S=S+Q*X(I+M)
        V(I)=S
100 CONTINUE
      RETURN
      END
      SUBROUTINE A25RQM(N,X,EPS,KPR,Y,Z,T,G,A,B,PO,IPR,APR,BPR)
C ALGORITHM 25 RAYLEIGH QUOTIENT MINIMIZATION BY CONJUGATE GRADIENTS
C J.C. NASH JULY 1978, FEBRUARY 1980, APRIL 1989
C N = ORDER OF PROBLEM
C X = INITIAL (APPROXIMATE?) EIGENVECTOR
C EPS = MACHINE PRECISION
C&&& for Microsoft test replace with actual names
C APR,BPR ARE NAMES OF SUBROUTINES WHICH FORM THE PRODUCTS
C V= A*X VIA CALL APR(N,X,V)
C T= B*X VIA CALL BPR(N,X,T)
C KPR = LIMIT ON THE NUMBER OF PRODUCTS (INPUT) (TAKES ROLE OF IPR)
C = PRODUCTS USED (OUTPUT)
C Y,Z,T,G,A,B RE WORKING VECTORS IN AT LEAST N ELEMENTS

```

```

C  PO  =  APPROXIMATE EIGENVALUE (OUTPUT)
C  IPR  =  PRINT CHANNEL   PRINTING IF IPR.GT.0
C  STEP 0
      INTEGER N,LP,IPR,ITN,I,LIM,COUNT
      REAL X(N),T(N),G(N),Y(N),Z(N),PN,A(N),B(N)
      REAL EPS,TOL,PO,PA,XAX,GBX,XAT,XBT,TAT,TBT,W,K,D,V,GG,BETA,TABT,U
C  IBM VALUE - APPROX. LARGEST NUMBER REPRESENTABLE.
C&&&      PA=R1MACH(2)
      PA=1E+35
      LIM=KPR
      KPR=0
      TOL=N*N*EPS*EPS
C  STEP 1
10  KPR=KPR+1
      IF(KPR.GT.LIM)RETURN
C  FIND LIMIT IN ORIGINAL PROGRAMS
      CALL APR(N,X,A)
      CALL BPR(N,X,B)
C  STEP 2
      XAX=0.0
      GBX=0.0
      DO 25 I=1,N
          XAX=XAX+X(I)*A(I)
          GBX=GBX+X(I)*B(I)
25  CONTINUE
C  STEP 3
      IF(GBX.LT.TOL)STOP
C  STEP 4
      PO=XAX/GBX
      IF(PO.GE.PA)RETURN
      IF(IPR.GT.0)WRITE(IPR,963)KPR,PO
963  FORMAT( 1H ,I4, ' PRODUCTS, EST. EIGENVALUE=',1PE16.8)
C  STEP 5
      PA=PO
C  STEP 6
      GG=0.0
      DO 65 I=1,N
          G(I)=2.0*(A(I)-PO*B(I))/GBX
          GG=GG+G(I)**2
65  CONTINUE
C  STEP 7
      IF(IPR.GT.0)WRITE(IPR,964)GG
964  FORMAT(' GRADIENT NORM SQUARED=',1PE16.8)
      IF(GG.LT.TOL)RETURN
C  STEP 8
      DO 85 I=1,N
          T(I)=-G(I)
85  CONTINUE
C  STEP 9
      DO 240 ITN=1,N
C  STEP 10
          KPR=KPR+1
          IF(KPR.GT.LIM)RETURN

```

```

        CALL APR(N,T,Y)
        CALL BPR(N,T,Z)
C  STEP 11
        TAT=0.0
        TBT=0.0
        XAT=0.0
        XBT=0.0
        DO 115 I=1,N
            TAT=TAT+T(I)*Y(I)
            XAT=XAT+X(I)*Y(I)
            TBT=TBT+T(I)*Z(I)
            XBT=XBT+X(I)*Z(I)
115     CONTINUE
C  STEP 12
        U=TAT*XBT-XAT*TBT
        V=TAT*XBX-XAX*TBT
        W=XAT*XBX-XAX*XBT
        D=V*V-4.0*U*W
C  STEP 13
        IF(D.LT.0)STOP
C  MAY NOT WISH TO STOP
C  STEP 14
        D=SQRT(D)
        IF(V.GT.0.0)GOTO 145
        K=0.5*(D-V)/U
        GOTO 150
145     K=-2.0*W/(D+V)
150     COUNT=0
C  STEP 15
        XAX=0.0
        XBX=0.0
        DO 155 I=1,N
            A(I)=A(I)+K*Y(I)
            B(I)=B(I)+K*Z(I)
            W=X(I)
            X(I)=W+K*T(I)
            IF(W.EQ.X(I))COUNT=COUNT+1
            XAX=XAX+X(I)*A(I)
            XBX=XBX+X(I)*B(I)
155     CONTINUE
C  STEP 16
        IF(XBX.LT.TOL)STOP
        PN=XAX/XBX
C  STEP 17
        IF(COUNT.LT.N)GOTO 180
        IF(ITN.EQ.1)RETURN
        GOTO 10
C  STEP 18
180     IF(PN.LT.P0)GOTO 190
        IF(ITN.EQ.1)RETURN
        GOTO 10
C  STEP 19
190     P0=PN

```

```

        GG=0.0
        DO 195 I=1,N
          G(I)=2.0*(A(I)-PN*B(I))/XBX
          GG=GG+G(I)**2
195     CONTINUE
C  STEP 20
        IF(GG.LT.TOL)GOTO 10
C  STEP 21
        XBT=0.0
        DO 215 I=1,N
          XBT=XBT+X(I)*Z(I)
215     CONTINUE
C  STEP 22
        TABT=0.0
        BETA=0.0
        DO 225 I=1,N
          W=Y(I)-PN*Z(I)
          TABT=TABT+T(I)*W
          BETA=BETA+G(I)*(W-G(I)*XBT)
225     CONTINUE
C  STEP 23
        BETA=BETA/TABT
        DO 235 I=1,N
          T(I)=BETA*T(I)-G(I)
235     CONTINUE
C  STEP 24
240    CONTINUE
C  STEP 25
        GOTO 10
C  NO STEP 26 - HAVE USED RETURN INSTEAD
        END

```

Example output

?? explanation needed

```

gfortran ../fortran/a25.f
mv ./a.out ../fortran/a25.run
../fortran/a25.run < ../fortran/a25.in

```

```

##  GRID ORDER   3  EQNS ORDER   9  LIMIT= 100
##    1 PRODUCTS, EST. EIGENVALUE=  1.33333337E+00
##  GRADIENT NORM SQUARED=  1.77777791E+00
##    5 PRODUCTS, EST. EIGENVALUE=  1.17157304E+00
##  GRADIENT NORM SQUARED=  5.56937471E-13
##  RETURNED AFTER   5 PRODUCTS WITH EV=  1.17157304E+00
##  RESIDUAL NORM=  1.31790827E-07 /  3.43119442E-01=  3.84096069E-07
##  GRID ORDER  10  EQNS ORDER  100  LIMIT= 400
##    1 PRODUCTS, EST. EIGENVALUE=  4.00000244E-01
##  GRADIENT NORM SQUARED=  1.28000033E+00
##   15 PRODUCTS, EST. EIGENVALUE=  1.62028164E-01
##  GRADIENT NORM SQUARED=  7.54772778E-09
##  RETURNED AFTER  15 PRODUCTS WITH EV=  1.62028164E-01
##  RESIDUAL NORM=  5.59246428E-06 /  1.13465175E-01=  4.92879371E-05
##  GRID ORDER  -1  EQNS ORDER   1  LIMIT=  0

```

Pascal

Listing

```
program dr25(input, output);
{dr25.pas == eigensolutions by minimisation of the Rayleigh quotient

    Copyright 1988 J.C.Nash
}
{constype.def ==
    This file contains various definitions and type statements which are
    used throughout the collection of "Compact Numerical Methods". In many
    cases not all definitions are needed, and users with very tight memory
    constraints may wish to remove some of the lines of this file when
    compiling certain programs.

    Modified for Turbo Pascal 5.0

    Copyright 1988, 1990 J.C.Nash
}
uses Dos, Crt; {Turbo Pascal 5.0 Modules}
{ 1. Interrupt, Unit, Interface, Implementation, Uses are reserved words now.}
{ 2. System,Dos,Crt are standard unit names in Turbo 5.0.}

const
    big = 1.0E+35;    {a very large number}
    Maxconst = 25;    {Maximum number of constants in data record}
    Maxobs = 100;     {Maximum number of observations in data record}
    Maxparm = 25;     {Maximum number of parameters to adjust}
    Maxvars = 10;     {Maximum number of variables in data record}
    acctol = 0.0001;  {acceptable point tolerance for minimisation codes}
    maxm = 20;        {Maximum number or rows in a matrix}
    maxn = 20;        {Maximum number of columns in a matrix}
    maxmn = 40;       {maxn+maxm, the number of rows in a working array}
    maxsym = 210;     {maximum number of elements of a symmetric matrix
        which need to be stored = maxm * (maxm + 1)/2 }
    reltest = 10.0;   {a relative size used to check equality of numbers.
        Numbers x and y are considered equal if the
        floating-point representation of reltest*x equals
        that of reltest*y.}
    stepredn = 0.2;   {factor to reduce stepsize in line search}
    yearwrit = 1990;  {year in which file was written}

type
    str2 = string[2];
    rmatrix = array[1..maxm, 1..maxn] of real; {a real matrix}
    wmatrix = array[1..maxmn, 1..maxn] of real; {a working array, formed
        as one real matrix stacked on another}
    smatvec = array[1..maxsym] of real; {a vector to store a symmetric matrix
        as the row-wise expansion of its lower triangle}
    rvector = array[1..maxm] of real; {a real vector. We will use vectors
        of m elements always. While this is NOT space efficient,
        it simplifies program codes.}
    cgmethodtype= (Fletcher_Reeves,Polak_Ribiere,Beale_Sorenson);
```

```

    {three possible forms of the conjugate gradients updating formulae}
  probdata = record
    m      : integer; {number of observations}
    nvar   : integer; {number of variables}
    nconst : integer; {number of constants}
    vconst : array[1..Maxconst] of real;
    Ydata  : array[1..Maxobs, 1..Maxvars] of real;
    nlls   : boolean; {true if problem is nonlinear least squares}
  end;
{
  NOTE: Pascal does not let us define the work-space for the function
  within the user-defined code. This is a weakness of Pascal for this
  type of work.
}
var {global definitions}
  banner      : string[80]; {program name and description}

function calceps:real;
{calceps.pas ==
  This function returns the machine EPSILON or floating point tolerance,
  the smallest positive real number such that 1.0 + EPSILON > 1.0.
  EPSILON is needed to set various tolerances for different algorithms.
  While it could be entered as a constant, I prefer to calculate it, since
  users tend to move software between machines without paying attention to
  the computing environment. Note that more complete routines exist.
}
var
  e,e0: real;
  i: integer;
begin {calculate machine epsilon}
  e0 := 1; i:=0;
  repeat
    e0 := e0/2; e := 1+e0; i := i+1;
  until (e=1.0) or (i=50); {note safety check}
  e0 := e0*2;
{ Writeln('Machine EPSILON =',e0);}
  calceps:=e0;
end; {calceps}

{$I matrixin.pas}
{$I vectorin.pas}

procedure matmul(nn : integer; {order of matrix}
  matrix: rmatrix;{the matrix or order nn}
  vectorin: rvector;{vector which is multiplied}
  var vectorout: rvector); {product vector}
{matmul.pas == Here we use an explicit matrix multiplication. This may
  be replaced by implicit forms as appropriate.}
var
  ii, jj : integer;
  tt : real;
begin
  for ii := 1 to nn do

```



```

begin
  tt := 0.0;
  for jj := 1 to nn do tt := tt+matrix[ii,jj]*vectorin[jj];
  vectorout[ii] := tt;
end; {loop on ii}
end; {matmul.pas}

procedure rqmcg( n : integer;
  A, B : rmatrix;
  var X : rvector;
  var ipr : integer;
  var rq : real);

var
  count, i, itn, itlimit : integer;
  avec, bvec, yvec, zvec, g, t : rvector;
  beta, d, eps, g2, gg, oldg2, pa, pn, s2, step : real;
  t2, ta, tabt, tat, tb, tbt, tol, u, v, w, xat, xax, xbt, xbx : real;
  conv, fail : boolean;

begin
  writeln('alg25.pas -- Rayleigh quotient minimisation');
  itlimit := ipr;
  fail := false;
  conv := false;
  ipr := 0;
  eps := calceps;
  tol := n*n*eps*eps;

  pa := big;
  while (ipr<=itlimit) and (not conv) do
    begin
      matmul(n, A, X, avec);
      matmul(n, B, X, bvec);
      ipr := ipr+1;

      xax := 0.0; xbx := 0.0;
      for i := 1 to n do
        begin
          xax := xax+X[i]*avec[i]; xbx := xbx+X[i]*bvec[i];
        end;
      if xbx<=tol then halt;
      rq := xax/xbx;
      write(ipr, ' products -- ev approx. =',rq:18);
      if rq<pa then
        begin
          pa := rq;
          gg := 0.0;
          for i := 1 to n do
            begin
              g[i] := 2.0*(avec[i]-rq*bvec[i])/xbx; gg := gg+g[i]*g[i];
            end;

```

```

writeln(' squared gradient norm =',gg:8);
if gg>tol then

begin

  for i := 1 to n do t[i] := -g[i];
  itn := 0;
  repeat
    itn := itn+1;
    matmul(n, A, t, yvec);
    matmul(n, B, t, zvec); ipr := ipr+1;
    tat := 0.0; tbt := 0.0; xat := 0.0; xbt := 0.0;
    for i := 1 to n do
      begin
        xat := xat+X[i]*yvec[i]; tat := tat+t[i]*yvec[i];
        xbt := xbt+X[i]*zvec[i]; tbt := tbt+t[i]*zvec[i];
      end;

    u := tat*xbt-xat*tbt; v := tat*xbx-xax*tbt;
    w := xat*xbx-xax*xbt; d := v*v-4.0*u*w;
    if d<0.0 then halt;

    d := sqrt(d);
    if v>0.0 then step := -2.0*w/(v+d) else step := 0.5*(d-v)/u;

    count := 0;
    xax := 0.0; xbx := 0.0;
    for i := 1 to n do
      begin
        avec[i] := avec[i]+step*yvec[i];
        bvec[i] := bvec[i]+step*zvec[i];
        w := X[i]; X[i] := w+step*t[i];
        if (reltest+w)=(reltest+X[i]) then count := count+1;
        xax := xax+X[i]*avec[i]; xbx := xbx+X[i]*bvec[i];
      end;
    if xbx<=tol then halt
      else pn := xax/xbx;
    if (count<n) and (pn<rq) then
      begin
        rq := pn; gg := 0.0;
        for i := 1 to n do
          begin
            g[i] := 2.0*(avec[i]-pn*bvec[i])/xbx; gg := gg+g[i]*g[i];
          end;
        if gg>tol then
          begin
            xbt := 0.0; for i := 1 to n do xbt := xbt+X[i]*zvec[i];

            tabt := 0.0; beta := 0.0;
            for i := 1 to n do
              begin
                w := yvec[i]-pn*zvec[i]; tabt := tabt+t[i]*w;
                beta := beta+g[i]*(w-g[i]*xbt);
              end;
          end;
        end;
      end;
  until itn>=itmax;
end;

```

```

        end;
        beta := beta/tabt;

        for i := 1 to n do t[i] := beta*t[i]-g[i];
        end;
    end

    else
    begin
        if itn=1 then conv := true;
        itn := n+1;
        end;
        until (itn>=n) or (count=n) or (gg<=tol) or conv;
    end
    else conv := true;
end
else
begin
    conv := true;
end;
ta := 0.0;
for i := 1 to n do ta := ta+sqr(X[i]); ta := 1.0/sqrt(ta);
for i := 1 to n do X[i] := ta*X[i];
end;
if ipr>itlimit then ipr := -ipr;
writeln;
end;

function resids(nRow, nCol: integer; A : rmatrix;
                Y: rvector; Bvec : rvector; print : boolean):real;
{resids.pas
== Computes residuals and , if print is TRUE, displays them 7
per line for the linear least squares problem. The sum of
squared residuals is returned.

    residual vector = A * Bvec - Y
}
var
i, j: integer;
t1, ss : real;

begin
    if print then
    begin
        writeln('Residuals');
    end;
    ss:=0.0;
    for i:=1 to nRow do
    begin
        t1:=-Y[i]; {note form of residual is residual = A * B - Y }
        for j:=1 to nCol do
            t1:=t1+A[i,j]*Bvec[j];
            ss:=ss+t1*t1;

```

```

    if print then
    begin
        write(t1:10,' ');
        if (i = 7 * (i div 7)) and (i<nRow) then writeln;
    end;
end; {loop on i}
if print then
begin
    writeln;
    writeln('Sum of squared residuals =',ss);
end;
resids:=ss
end; {resids.pas == residual calculation for linear least squares}

var
    A, B : rmatrix;
    X : rvector; {eigenvector}
    Y : rvector; {for residuals}
    avec : smatvec; {for matrixin only}
    sym : boolean; {to tell if matrix symmetric}
    ch : char;
    i, j, n, itcount : integer;
    ev, t, s : real;

begin
    banner:='dr25.pas -- minimise Rayleigh quotient';
    write('Order of problem =');
    readln(n); writeln(n);
    writeln('Matrix A');
??
    matrixin(n, n, A, avec, sym);
    if not sym then
    begin
        writeln('Matrix not symmetric -- halting');
        halt;
    end;
??
    writeln('Metric matrix B');
    matrixin(n, n, B, avec, sym);
?? if not sym then
    begin
        writeln('Matrix not symmetric -- halting');
        writeln(confile,'Matrix not symmetric -- halting');
        halt;
    end;
??
    writeln('Initial eigenvector approximation');
?? vectorin(n, X);
    itcount:=100*n; {safety setting}
    rqmcg( n, A, B, X, itcount, ev);
    writeln('Solution after ',itcount,' products. Est. eigenvalue =',ev);
    for i:=1 to n do

```

```

begin
  write(X[i]:10:7,' ');
  if (7 * (i div 7) = i) and (i<n) then writeln;
  t:=0.0;
  for j:=1 to n do t:=t+B[i,j]*X[j];
  Y[i]:=ev*t; {to save eigenvalue * matrix-vector product for residuals}
end;
writeln;
s := resids(n, n, A, Y, X, true);
end. {dr25.pas}

```

Example output

?? not yet working

Cleanup of working files

The following script is included to remove files created during compilation or execution of the examples.

```

## remove object and run files
cd ../fortran/
echo `pwd`
rm *.o
rm *.run
# rm *.out
cd ../Pascal2021/
echo `pwd`
rm *.o
rm *.run
# rm *.out
cd ../BASIC
echo `pwd`
# rm *.out
cd ../Documentation
## ?? others

## /j19z/j19store/versioned/Nash-Compact-Numerical-Methods/fortran
## rm: cannot remove '*.o': No such file or directory
## /j19z/j19store/versioned/Nash-Compact-Numerical-Methods/Pascal2021
## /j19z/j19store/versioned/Nash-Compact-Numerical-Methods/BASIC

```

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